1. INTRODUCTION TO APPROXIMATION

Approximation is a numerical procedure of calculating fairly accurate values of a function $f(x)$ by using corresponding approximation function suitable for numerical manipulation. For example, a lot of functions, such as logarithmic and trigonometric functions, whose values cannot be calculated directly, are approximated with the corresponding power series. These power series when once determined are forever. The most important ones are included in the standard computers' mathematical libraries and implemented in the hardware of scientific calculators.

Let function $f(x)$ be approximated by *approximation function*

$$\tilde{f}(x,\beta) = \tilde{f}(x,\beta_0,\beta_1,...,\beta_{N-1}) , \tag{1.1}$$

so that the *approximation error* (usually called *residual*) defined as a difference between function $f(x)$ and its approximation $\tilde{f}(x,\beta)$ is minimised on the chosen domain by the appropriate choice of the coefficients β_n $(n = 0,1,...,N-1)$.

Depending on whether a domain on which the approximation is provided is continuous or discrete, the approximation is of *continuous type* or *discrete type*.

In the approximation of continuous type the approximated function $f(x)$ and the approximation error

$$E(x,\beta) = E(x,\beta_0,\beta_1,...,\beta_{N-1}) = f(x) - \tilde{f}(x,\beta) , \tag{1.2}$$

are defined on a continuous domain.

In the approximation of discrete type an approximated function $f(x)$ is defined on a discrete domain by its values $f^k = f(\xi^k)$ in a chosen set of distinct points ξ^k, called *sampling points* or *nodes*[1]. In this case, the approximation error is also defined as the difference between value f^k of approximated function $f(x)$ and its approximation $\tilde{f}(\xi^k, \beta)$ in the sampling point ξ^k, as

$$E(\xi^k, \beta) = E(\xi^k, \beta_0, \beta_1, ..., \beta_{N-1}) = f^k - \tilde{f}(\xi^k, \beta) . \tag{1.3}$$

Furthermore, the approximation can be of linear and nonlinear type. In the *approximation of linear type* approximation function $\tilde{f}(x,\beta)$ is a *linear combination* of so called *coordinate functions* $\phi_n(x)$ and can be expressed by the *approximation formula*:

$$\tilde{f}(x, \beta) = \sum_{n=0}^{N-1} \beta_n \phi_n(x) = \beta_0 \phi_0(x) + \beta_1 \phi_1(x) + ... + \beta_{N-1} \phi_{N-1}(x) . \tag{1.4}$$

Used set of coordinate functions $\{\phi_n(x)\}$ can be chosen arbitrary as long as it is *complete*[2] and *linearly independent*[3].

If the function $f(x) = f(x(x_1, x_2,..., x_M))$ depends on *M* arguments x_m, then by substitutions

$$\begin{aligned} &n = n(n_1, n_2,..., n_M) \quad \text{(unique } n \text{ for each combination of } n_1, n_2,..., n_M\text{)}, \\ &\beta_n = \beta_{n(n_1 n_2 ... n_M)} = \beta_{n_1 n_2 ... n_M} , \\ &\phi_n(x) = \phi_{n(n_1 n_2 ... n_M)}(x(x_1, x_2,..., x_M)) = \phi^{[1]}_{n_1}(x_1) \phi^{[2]}_{n_2}(x_2) ... \phi^{[M]}_{n_M}(x_M), \end{aligned} \tag{1.5}$$

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[1] Note that upper index *k* is an index of a function value f^k and sampling point ξ^k and *not* an exponent. Lower index denotes coordinates ξ^k_1, ξ^k_2, … of a sampling point ξ^k.

[2] The set of functions $\{1, x, x^2,..., x^{N-1}\}$ is *complete* with respect to any approximated function, while the set of functions $\{x, x^2,..., x^{N-1}\}$ is complete only if $f(0) = 0$, since $\tilde{f}(x, \beta) = \beta_1 x + \beta_2 x^2 + ... + \beta_{N-1} x^{N-1}$ cannot approximate function that has non zero value at $x = 0$.

[3] Consider that functions $\phi_n(x)$ are *linearly dependent*, i.e. that at least one of them can be expressed as a linear combination of others as $\phi_L = \sum_{n \neq L} \alpha_n \phi_n$. Substitution of ϕ_L into original approximation formula (1.4) yields to the approximation formula of the same form $\tilde{f}(x, \bar{\beta}) = \sum_n \bar{\beta}_n \phi_n(x)$ in which $\bar{\beta}_n = \beta_n + \beta_L \alpha_n$ ($n \neq L$) and $\bar{\beta}_L = 0$, i.e. to the approximation formula in which the linearly depended function ϕ_L is excluded.

the approximation formula $\tilde{f}(x,\beta) = \sum_{n=0}^{N-1} \beta_n \phi_n(x)$ can also be expressed in the equivalent (but expanded) form

$$\tilde{f}(x,\beta) = \sum_{n_1=0}^{N_1-1} \sum_{n_2=0}^{N_2-1} \cdots \sum_{n_M=0}^{N_M-1} \beta_{n_1 n_2 \ldots n_M} \phi_{n_1}^{[1]}(x_1) \phi_{n_2}^{[2]}(x_2) \ldots \phi_{n_M}^{[M]}(x_M)\,. \tag{1.6}$$

Coordinate functions $\phi_{n_1}^{[1]}(x_1)$, $\phi_{n_2}^{[2]}(x_2)$, … are usually chosen from the same family of functions $\{\phi_n^*\}$. In this case

$$\tilde{f}(x,\beta) = \sum_{n_1=0}^{N_1-1} \sum_{n_2=0}^{N_2-1} \cdots \sum_{n_M=0}^{N_M-1} \beta_{n_1 n_2 \ldots n_M} \phi_{n_1}^*(x_1)\, \phi_{n_2}^*(x_2) \ldots \phi_{n_M}^*(x_M)\,. \tag{1.7}$$

The approximations of linear type are relatively simple in comparison to the approximations of nonlinear type, and for that reason are frequently used. The approximations of nonlinear type in which nonlinear combinations of coordinate functions are involved, like most nonlinear analysis, are difficult to be formulated and applied and because of that are rarely used. However, the exception is the nonlinear *approximation of real type* which has the form

$$\tilde{f}(x,a,b) = \frac{\sum_{n_1=0}^{N_1-1} a_{n_1} \phi_{n_1}(x)}{\sum_{n_2=0}^{N_2-1} b_{n_2} \phi_{n_2}(x)}\,, \tag{1.8}$$

where a_{n_1} and b_{n_2} are constant parameters.

Although coordinate functions $\phi_n(x)$ can be chosen arbitrary, it is usually more convenient to expand the function $f(x)$ into infinite series

$$f(x) = \sum_{n=0}^{\infty} \beta_n \phi_n(x)\,, \tag{1.9}$$

such as

1. Taylor series,
2. Maclaurin series (special case of Taylor series),
3. series of orthogonal functions (e.g. Fourier series),
4. series of orthogonal polynomials.

Approximation function $\tilde{f}(x,\beta)$ is then a partial sum of the first *N* elements

$$S_N(x,\beta) = \sum_{n=0}^{N-1} \beta_n \phi_n(x) \qquad (1.10)$$

that is compliant with (1.4).

The crux of the approximation problem is a criterion of minimising approximation error that will determine constants β_n. The five major methods of doing this lead to the five main types of approximations which are of the highest importance:

1. *Approximation near the point* in which the approximation and its first derivatives are equal to the approximated function $f(x)$ and its first derivatives $f^{(n)}(x)$ in the single point $x = \xi$:
    a. *Taylor series expansion*: series of powers $(x-\xi)^k$ whose partial sum $S_N(x,\beta) = \beta_0 + \beta_1(x-\xi) + ... + \beta_{N-1}(x-\xi)^{N-1}$ and its first $N-1$ derivatives $S_N^{(n)}(x,\beta)$ are equal to the approximated function $f(x)$ and its first $N-1$ derivatives $f^{(n)}(x)$ in the chosen point $x = \xi$; precisely, $f(\xi) = S_N(\xi,\beta)$ and $f^{(n)}(\xi) = S_N^{(n)}(\xi,\beta)$ for $n = 1,...,N-1$.
    b. *Maclaurin series expansion*: series of powers x^k whose partial sum $S_N(x,\beta) = \beta_0 + \beta_1 x + ... + \beta_{N-1}x^{N-1}$ and its first $N-1$ derivatives $S_N^{(n)}(x,\beta)$ are equal to the approximated function $f(x)$ and its first $N-1$ derivatives $f^{(n)}(x)$ in the point $x = 0$; precisely, $f(0) = S_N(0,\beta)$ and $f^{(n)}(0) = S_N^{(n)}(0,\beta)$ for $n = 1,...,N-1$.
    c. *Padé approximation*: the rational function $R_{nm}(x)$ defined as a quotient of two polynomials $P_n(x)/Q_m(x)$ of orders *n* and *m*, whose value and the values of its first $n+m$ derivatives $R_{nm}^{(k)}(x)$, $k = 1,...,n+m$, equals to the exact values of the approximated function $f(x)$ and its first $n+m$ derivatives $f^{(k)}(x)$ at the point $x = \xi$; precisely, $f(\xi) = R_{nm}(\xi)$ and $f^{(k)}(\xi) = R_{nm}^{(k)}(\xi)$ for $k = 1,...,n+m$.

2. *Exact* or *interpolatory approximation*:
   a. *Interpolation*, in which the constants β_n are chosen so that the approximation $\tilde{f}(\xi^k, \beta)$ equals to the values of function $f^k = f(\xi^k)$ in the chosen set of *K* distinct points ξ^k, $k = 1, ..., K$.
   b. *Hermite interpolation*, in which the approximation $\tilde{f}(\xi^k, \beta)$ and its first derivatives $\tilde{f}^{(n)}(\xi^k, \beta)$ (where *n* is positive integer) equals to the values of function $f(\xi^k)$ and its first derivatives $f^{(n)}(\xi^k)$ in the chosen set of *K* distinct points ξ^k, $k = 1, ..., K$.

3. *Least-squares approximation*:
   a. *Continuous least-squares approximation,* in which the goal is to minimise the integral of the squared approximation error $[f(x) - \tilde{f}(x, \beta)]^2$ (optionally multiplied by *weighting function*) over a given continuous domain.
   b. *Discrete least-squares approximation*, in which the goal is to minimise the sum of the squared approximation error $[f(\xi^k) - \tilde{f}(\xi^k, \beta)]^2$ (optionally multiplied by *weighting coefficients*) over a discrete set of *K* distinct points ξ^k.

   The Fourier series and series of orthogonal functions inherently satisfy *least-squares* criteria.

4. *Uniform or minimum-maximum approximation*:
   a. *Continuous uniform approximation,* in which the aim is to minimise the maximum magnitude of the approximation error $\max|f(x) - \tilde{f}(x, \beta)|$ (optionally multiplied by *weighting function*) on a continuous domain.
   b. *Discrete uniform approximation*, in which the aim is to minimise the maximum magnitude of the approximation error $\max|f(\xi^k) - \tilde{f}(\xi^k, \beta)|$ (optionally multiplied by *weighting coefficients*) over a discrete set of *K* distinct points ξ^k.

5. Approximation and interpolation by *splines* consists in splitting an interval into segments on which the approximations or interpolations are provided separately, while the approximation function $\tilde{f}(\xi^k, \beta)$ and its first derivatives $\tilde{f}^{(n)}(\xi^k, \beta)$ have equal values on the shared boundary points ξ^k of joined segments.

1.1 APPROXIMATION NEAR THE POINT

In this type of approximations, the values of approximation and its first derivatives are equal to the values of the approximated function and its first derivatives in the single approximation point. Although approximation error is small in the area close to the approximation point, it increases rapidly away from that point.

1.1.1 Taylor series expansion

The function $f(x)$ of single argument x can be expanded into infinite power series

$$f(x)=\sum_{n=1}^{\infty}\beta_n(x-\xi)^n=\beta_0+\beta_1(x-\xi)+\beta_2(x-\xi)^2+\beta_3(x-\xi)^3+\dots . \quad (1.11)$$

If the function $f(x)$ has derivatives of all orders on an interval containing the points x and ξ, the coefficients $\beta_0, \beta_1, \dots$ can be determined by the conditions

$$\begin{aligned} & f(\xi)=\beta_0, \\ & \frac{\mathrm{d}^n f(\xi)}{\mathrm{d}x^n}=n!\,\beta_n, \quad n \geq 1. \end{aligned} \quad (1.12)$$

So obtained power series in ($x-\xi$) of the form

$$f(x)=f(\xi)+\sum_{n=1}^{\infty}\frac{\mathrm{d}^n f(\xi)}{\mathrm{d}x^n}\frac{(x-\xi)^n}{n!}, \quad (1.13)$$

is called the *Taylor series expansion* of function $f(x)$ in the point ξ [1].

By introducing notation

$$\begin{aligned} & f^{(0)}(\xi)=f(\xi), \\ & f^{(n)}(\xi)=\frac{d^n f(\xi)}{dx^n}, \quad n \geq 1, \end{aligned} \quad (1.14)$$

the Taylor formula (1.13) can be expressed in a simpler form

$$f(x)=\sum_{n=0}^{\infty}f^{(n)}(\xi)\frac{(x-\xi)^n}{n!}. \quad (1.15)$$

Example 1.1. Taylor series expansion of the function $\ln(x)$ in the point $\xi = 1$

$$\ln(x) = (x-1) - \frac{(x-1)^2}{2} + \frac{(x-1)^3}{3} - \frac{(x-1)^4}{4} + \dots, \quad 0 < x \le 2 \,. \tag{1.16}$$

Function $f(x)$ can be approximated by the first N terms of the Taylor series as

$$\tilde{f}(x) = S_N(x) = \sum_{n=0}^{N-1} f^{(n)}(\xi)\frac{(x-\xi)^n}{n!} \,. \tag{1.17}$$

This formula is equivalent to the approximation formula (1.4). Precisely

$$\tilde{f}(x, \beta) = \sum_{n=0}^{N-1} \beta_n \phi_n(x, \xi) \,, \tag{1.18}$$

where

$$\begin{aligned} \beta_n &= \frac{f^{(n)}(\xi)}{n!}, \qquad n \ge 0, \\ \phi_n(x,\xi) &= (x-\xi)^n, \quad n \ge 0. \end{aligned} \tag{1.19}$$

The approximation error in the integral form is [2]:

$$\begin{aligned} E_N(x) = f(x) - S_N(x) &= \frac{1}{(N-1)!}\int_{\xi}^{x} f^{(N)}(\xi)(x-\xi)^{N-1}\mathrm{d}\xi \\ &= N\int_{\xi}^{x} \beta_N(\xi)\,\phi_{N-1}(x,\xi)\,\mathrm{d}\xi. \end{aligned} \tag{1.20}$$

By the use of a mean theorem of calculus which says

$$\int_{\xi}^{x} f^{(N)}(\xi)(x-\xi)^{N-1}\mathrm{d}\xi = f^{(N)}(\zeta)\int_{\xi}^{x}(x-\xi)^{N-1}\mathrm{d}\xi \,, \tag{1.21}$$

where ζ is a point between ξ and x, otherwise unknown, the approximation error can be obtained in the Lagrange form

$$E_N(x) = \frac{f^{(N)}(\zeta)}{N!}(x-\xi)^N \quad \text{or} \quad E_N(x) = \beta_N(\zeta)\,\phi_N(x,\xi) \,. \tag{1.22}$$

This form of the error is very popular because of its close similarity to the terms of the Taylor polynomial. Except for a ζ in the place of a ξ it would be a term which produces the Taylor polynomial of the next higher degree.

At the point $x = \xi$, the approximation $\tilde{f}(\xi) = f(\xi)$ has no error, since $(x-\xi)^n = 0$ for $x = \xi$ and $n \geq 1$.

The Taylor series expansion can also be applied in multiple dimension domains.

In a two dimensional domain the function $f(x)$ depends on two coordinates x_1 and x_2 of the point $x(x_1, x_2)$. The function $f(x) = f(x_1, x_2)$ of two arguments x_1 and x_2 can be expanded into infinite power series

$$f(x) = \sum_{n_1=1}^{\infty}\sum_{n_2=1}^{\infty} \beta_{n_1 n_2} (x_1 - \xi_1)^{n_1} (x_2 - \xi_2)^{n_2} \ . \tag{1.23}$$

If the function $f(x)$ has derivatives of all orders on a domain containing the points $x(x_1, x_2)$ and $\xi(\xi_1, \xi_2)$, the coefficients $\beta_{n_1 n_2}$ can be determined by the conditions

$$\begin{aligned}
&f(\xi) = \beta_{0,0}, \\
&\frac{\partial^{n_1} f(\xi)}{\partial x_1^{n_1}} = n_1!\beta_{n_1,0}, \qquad && n_1 \geq 1, \\
&\frac{\partial^{n_2} f(\xi)}{\partial x_2^{n_2}} = n_2!\beta_{0,n_2}, \qquad && n_2 \geq 1, \\
&\frac{\partial^{n_1+n_2} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2}} = n_1! n_2! \beta_{n_1 n_2}, \qquad && n_1 \geq 1, n_2 \geq 1.
\end{aligned} \tag{1.24}$$

Therefore, the expansion at the point $\xi(\xi_1, \xi_2)$ can be done by

$$\begin{aligned}
f(x) = f(\xi) &+ \sum_{n_1=1}^{\infty} \frac{\partial^{n_1} f(\xi)}{\partial x_1^{n_1}} \frac{(x_1 - \xi_1)^{n_1}}{n_1!} + \sum_{n_2=1}^{\infty} \frac{\partial^{n_2} f(\xi)}{\partial x_2^{n_2}} \frac{(x_2 - \xi_2)^{n_2}}{n_2!} + \\
&+ \sum_{n_1=1}^{\infty} \sum_{n_2=1}^{\infty} \frac{\partial^{n_1+n_2} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2}} \frac{(x_1 - \xi_1)^{n_1}}{n_1!} \frac{(x_2 - \xi_2)^{n_2}}{n_2!}.
\end{aligned} \tag{1.25}$$

It is convenient to define zero-derivative that is only formally a derivative as it leaves functions unchanged. I.e., if it is assumed that

$$\frac{\partial^{n_1+n_2} f(\xi)}{\partial x_1^{n_1}\partial x_2^{n_2}} = \begin{cases} f(\xi) & n_1 = 0,\ n_2 = 0, \\ \dfrac{\partial^{n_1}}{\partial x_1^{n_1}} f(\xi) & n_1 \geq 1,\ \ n_2 = 0, \\ \dfrac{\partial^{n_2}}{\partial x_2^{n_2}} f(\xi) & n_1 = 0,\ \ n_2 \geq 1, \end{cases} \tag{1.26}$$

then the Taylor formula for two arguments can be written in the short form

$$f(x) = \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty} \frac{\partial^{n_1+n_2} f(\xi)}{\partial x_1^{n_1}\partial x_2^{n_2}} \frac{(x_1-\xi_1)^{n_1}}{n_1!}\frac{(x_2-\xi_2)^{n_2}}{n_2!}. \tag{1.27}$$

The approximation can be made by using the approximation formula

$$\tilde{f}(x) = \sum_{n_1=0}^{N_1-1}\sum_{n_2=0}^{N_2-1} \frac{\partial^{n_1+n_2} f(\xi)}{\partial x_1^{n_1}\partial x_2^{n_2}} \frac{(x_1-\xi_1)^{n_1}}{n_1!}\frac{(x_2-\xi_2)^{n_2}}{n_2!}. \tag{1.28}$$

N_1 is a constant, while N_2 can be either a constant (usually $N_2 = N_1$) or a function of n_1. If N_2 is a constant, the approximation formula (1.28) has $N = N_1 N_2$ elements. If N_2 is a function of n_1, so that $N_2 = N_1 - n_1$, the approximation formula (1.28) has $N = N_1(N_1+1)/2$ elements.

Example 1.2. Double Taylor series expansion. For $N_1 = N_2 = 4$, the approximation formula (1.28) has 16 summation elements,

1	$(x_2-\xi_2)$	$(x_2-\xi_2)^2$	$(x_2-\xi_2)^3$
$(x_1-\xi_1)$	$(x_1-\xi_1)(x_2-\xi_2)$	$(x_1-\xi_1)(x_2-\xi_2)^2$	$(x_1-\xi_1)(x_2-\xi_2)^3$
$(x_1-\xi_1)^2$	$(x_1-\xi_1)^2(x_2-\xi_2)$	$(x_1-\xi_1)^2(x_2-\xi_2)^2$	$(x_1-\xi_1)^2(x_2-\xi_2)^3$
$(x_1-\xi_1)^3$	$(x_1-\xi_1)^3(x_2-\xi_2)$	$(x_1-\xi_1)^3(x_2-\xi_2)^2$	$(x_1-\xi_1)^3(x_2-\xi_2)^3$

while for $N_1 = 4$ and $N_2 = N_1 - n_1$ the approximation formula (1.28) has 10 summation elements

1	$(x_2-\xi_2)$	$(x_2-\xi_2)^2$	$(x_2-\xi_2)^3$
$(x_1-\xi_1)$	$(x_1-\xi_1)(x_2-\xi_2)$	$(x_1-\xi_1)(x_2-\xi_2)^2$	
$(x_1-\xi_1)^2$	$(x_1-\xi_1)^2(x_2-\xi_2)$		
$(x_1-\xi_1)^3$			

The Taylor formula (1.27) for expansion of a function of two arguments can be generalised to the formula for expansion of a function which has *M* arguments $x_1, x_2, \dots x_M$

$$f(x) = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \dots \sum_{n_M=0}^{\infty} \frac{\partial^{n_1+n_2+\dots+n_M} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2} \dots \partial x_M^{n_M}} \frac{(x_1-\xi_1)^{n_1}}{n_1!} \frac{(x_2-\xi_2)^{n_2}}{n_2!} \dots \frac{(x_M-\xi_M)^{n_M}}{n_M!}. \quad (1.29)$$

This formula is equivalent to

$$f(x) = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \dots \sum_{n_M=0}^{\infty} \beta_{n_1 n_2 \dots n_M} \phi_{n_1}^*(x_1) \phi_{n_1}^*(x_1) \dots \phi_{n_M}^*(x_M), \quad (1.30)$$

where

$$\beta_{n_1 n_2 \dots n_M} = \frac{1}{n_1! n_2! \dots n_M!} \frac{\partial^{n_1+n_2+\dots+n_M} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2} \dots \partial x_M^{n_M}},$$
$$\phi_{n_m}^*(x_m) = (x_m - \xi_m)^{n_m}, \quad n_m \geq 1, \quad m = 1, 2, \dots, M. \quad (1.31)$$

The approximation can be made by using the formula (1.7) with $N = N_1 N_2 \dots N_M$ elements.

1.1.2 Maclaurin series expansion

Maclaurin series can be obtained from the Taylor series by putting point ξ on the origin of the coordinate system ($\xi = 0$). The series in *x* of the form

$$f(x) = f(0) + \sum_{n=1}^{\infty} f^{(n)}(0) \frac{x^n}{n!} \quad (1.32)$$

is called the *Maclaurin series expansion* of the function $f(x)$ (upper index of x^n is an exponent).

Example 1.3. Few examples of *Maclaurin series expansion*:

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots, \quad (1.33)$$

$$\sin x = \frac{x}{1!} - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots, \quad (1.34)$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \dots, \quad (1.35)$$

$$\sinh x = \frac{x}{1!} + \frac{x^3}{3!} + \frac{x^5}{5!} + \frac{x^7}{7!} + \dots . \quad (1.36)$$

The function $f(x)$ can be approximated by the first N terms of series as

$$\tilde{f}(x) = \sum_{n=0}^{N-1} f^{(n)}(0)\frac{x^n}{n!} . \quad (1.37)$$

At the point $x = 0$, the approximated value of function $\tilde{f}(0) = f(0)$ is given without error since $x^n = 0$.

By analogy to the Taylor series expansion, the Maclaurin series expansion can also be applied on multiple dimension domains. For example, on a two dimensional domain, by putting $\xi_1 = 0$ and $\xi_2 = 0$ into (1.27) it is easy to obtain

$$f(x) = \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\frac{\partial^{n_1+n_2} f(0)}{\partial x_1^{n_1}\partial x_2^{n_2}}\frac{x_1^{n_1} x_2^{n_2}}{n_1! n_2!}. \quad (1.38)$$

Example 1.4. Maclaurin series expansion of $f(x_1, x_2) = e^{x_1+x_2}$. The derivatives are

$$\frac{\partial^{n_1+n_2} f(0,0)}{\partial x_1^{n_1}\partial x_2^{n_2}} = 1 . \quad (1.39)$$

From the expansion formula (1.38) follows

$$e^{x_1+x_2} = \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\frac{x_1^{n_1} x_2^{n_2}}{n_1! n_2!} = \left(\sum_{n_1=0}^{\infty}\frac{x_1^{n_1}}{n_1!}\right)\left(\sum_{n_2=0}^{\infty}\frac{x_2^{n_2}}{n_2!}\right). \quad (1.40)$$

The approximation can be made, say, by using the approximation formula with $N_1 N_2 = 4 \cdot 4 = 16$ summation elements,

$$e^{x_1+x_2} \approx \left(1 + x_1 + \frac{x_1^2}{2!} + \frac{x_1^3}{3!}\right)\left(1 + x_2 + \frac{x_2^2}{2!} + \frac{x_2^3}{3!}\right) \quad (1.41)$$

or, by using the approximation formula with $N_1(N_1 + 1)/2 = 10$ summation elements

$$e^{x_1+x_2} \approx 1 + \underbrace{x_1 + x_2}_{n_1+n_2=1} + \underbrace{\frac{x_1^2}{2!} + \frac{x_1}{1!}\frac{x_2}{1!} + \frac{x_2^2}{2!}}_{n_1+n_2=2} + \underbrace{\frac{x_1^3}{3!} + \frac{x_1^2}{2!}\frac{x_2}{1!} + \frac{x_1}{1!}\frac{x_2^2}{2!} + \frac{x_2^3}{3!}}_{n_1+n_2=3} \quad (1.42)$$

1.1.3 Padé approximant

The *Padé approximant* of order (*n*,*m*), $n \geq 0$, $m \geq 0$, is the rational function

$$R_{nm}(x) = \frac{P_n(x)}{Q_m(x)} = \frac{a_0 + a_1(x-\xi) + ... + a_n(x-\xi)^n}{b_0 + b_1(x-\xi) + ... + b_m(x-\xi)^m}, \tag{1.43}$$

where coefficients $a_0, a_1, ..., a_n$, $b_0, b_1, ..., b_m$ are determined by the conditions

$$\begin{aligned} &f(\xi) = R_{nm}(\xi), \\ &f^{(1)}(\xi) = R_{nm}^{(1)}(\xi), \\ &f^{(2)}(\xi) = R_{nm}^{(2)}(\xi), \\ &... \\ &f^{(n+m)}(\xi) = R_{nm}^{(n+m)}(\xi). \end{aligned} \tag{1.44}$$

Equivalently, if $R_{nm}(x)$ and $f(x)$ are both expanded in the Taylor series

$$\begin{aligned} R_{nm}(x) = f(\xi) + \frac{f^{(1)}(\xi)}{1!}(x-\xi) + ... + \frac{f^{(n+m)}(\xi)}{(n+m)!}(x-\xi)^{n+m} + \\ + \frac{R_{nm}^{(n+m+1)}(\xi)}{(m+n+1)!}(x-\xi)^{n+m+1} + ..., \end{aligned} \tag{1.45}$$

$$f(x) = f(\xi) + \frac{f^{(1)}(\xi)}{1!}(x-\xi) + \frac{f^{(2)}(\xi)}{2!}(x-\xi)^2 + ...,$$

the first $n+m+1$ terms of $R_{nm}(x)$ would cancel the first $n+m+1$ terms of $f(x)$, and as such the approximation error is

$$E(x) = f(x) - R_{nm}(x) = c_{n+m+1}(x-\xi)^{n+m+1} + c_{n+m+2}(x-\xi)^{n+m+2} + ... \tag{1.46}$$

The Padé approximant is unique for a given *n* and *m*, that is, the coefficients $a_0, a_1, ..., a_n$, $b_0, b_1, ..., b_m$, can be uniquely determined. It is for the reason of uniqueness that the zero order term b_0 at the denominator of $R_{nm}(x)$ is usually chosen to be 1.

Padé approximant is developed by Henri Padé. It often gives a better approximation of the function than truncating its Taylor (or Maclaurin) series, and may still work where the Taylor series does not converge.

Determination of coefficients a_i ($i \le n$) and b_j ($j \le m$) can begin from the equation system containing equation $R_{nm}(x)Q_m(x) = P_n(x)$ and its derivatives.

According to the formula (A.24) for multiple derivatives of products (see Appendix A.5)

$$\sum_{j=0}^{i} \frac{R_{nm}^{(i-j)}(x)}{(i-j)!} \frac{Q_m^{(j)}(x)}{j!} = \frac{P_n^{(i)}(x)}{i!}, \quad i = 0, 1, 2, \dots . \tag{1.47}$$

Upper index in the brackets denotes derivative, e.g. $P_n^{(2)}(x) \equiv P_n''(x)$. By the definition $R_{nm}^{(0)}(x) \equiv R_{nm}(x)$, $Q_m^{(0)}(x) \equiv Q_m(x)$ and $P_n^{(0)}(x) \equiv P_n(x)$.

Since $f^{(i)}(\xi) = R_{nm}^{(i)}(\xi)$ (1.44), and since derivatives of the polynomials at $x = \xi$ are $P_n^{(i)}(\xi) = i!a_i$ and $Q_m^{(j)}(\xi) = j!b_j$, from the equation (1.47) follows

$$\frac{f^{(i)}(\xi)}{i!} b_0 + \frac{f^{(i-1)}(\xi)}{(i-1)!} b_1 + \frac{f^{(i-2)}(\xi)}{(i-2)!} b_2 + \dots + \frac{f^{(0)}(\xi)}{0!} b_i = a_i . \tag{1.48}$$

The first *k* equations (1.48) can be written in the matrix form

$$\begin{bmatrix} \frac{f(\xi)}{0!} & 0 & 0 & 0 & \dots & 0 \\ \frac{f^{(1)}(\xi)}{1!} & \frac{f(\xi)}{0!} & 0 & 0 & \dots & 0 \\ \frac{f^{(2)}(\xi)}{2!} & \frac{f^{(1)}(\xi)}{1!} & \frac{f(\xi)}{0!} & 0 & \dots & 0 \\ \frac{f^{(3)}(\xi)}{3!} & \frac{f^{(2)}(\xi)}{2!} & \frac{f^{(1)}(\xi)}{1!} & \frac{f(\xi)}{0!} & \dots & 0 \\ \frac{f^{(4)}(\xi)}{4!} & \frac{f^{(3)}(\xi)}{3!} & \frac{f^{(2)}(\xi)}{2!} & \frac{f^{(1)}(\xi)}{1!} & \dots & 0 \\ \dots & \dots & \dots & \dots & & \dots \\ \frac{f^{(k)}(\xi)}{k!} & \frac{f^{(k-1)}(\xi)}{(k-1)!} & \frac{f^{(k-2)}(\xi)}{(k-2)!} & \frac{f^{(k-3)}(\xi)}{(k-3)!} & \dots & \frac{f(\xi)}{0!} \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ \dots \\ b_k \end{Bmatrix} = \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ \dots \\ a_k \end{Bmatrix}. \tag{1.49}$$

By putting $a_i = 0$ for $i > n$, $b_j = 0$ for $j > m$ and $b_0 = 1$ a linear equation system can be obtained whose solution are coefficients a_i ($i \le n$) and b_j ($j \le m$).

Example 1.5. Padé approximant. For $n = m = 2$ and $\xi = 0$, the equation system (1.49) reduces to

$$\begin{bmatrix} f(0) & 0 & 0 \\ f^{(1)}(0) & f(0) & 0 \\ \frac{1}{2} f^{(2)}(0) & f^{(1)}(0) & f(0) \\ \frac{1}{6} f^{(3)}(0) & \frac{1}{2} f^{(2)}(0) & f^{(1)}(0) \\ \frac{1}{24} f^{(4)}(0) & \frac{1}{6} f^{(3)}(0) & \frac{1}{2} f^{(2)}(0) \end{bmatrix} \begin{Bmatrix} 1 \\ b_1 \\ b_2 \end{Bmatrix} = \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ 0 \\ 0 \end{Bmatrix}. \tag{1.50}$$

This equation system can be divided into the two equation systems, the first one determining coefficients b_1 and b_2:

$$\begin{bmatrix} \frac{1}{6} f^{(3)}(0) & \frac{1}{2} f^{(2)}(0) & f^{(1)}(0) \\ \frac{1}{24} f^{(4)}(0) & \frac{1}{6} f^{(3)}(0) & \frac{1}{2} f^{(2)}(0) \end{bmatrix} \begin{Bmatrix} 1 \\ b_1 \\ b_2 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \tag{1.51}$$

and the second one determining coefficients a_0, a_1 and a_2:

$$\begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{bmatrix} f(0) & 0 & 0 \\ f^{(1)}(0) & f(0) & 0 \\ \frac{1}{2} f^{(2)}(0) & f^{(1)}(0) & f(0) \end{bmatrix} \begin{Bmatrix} 1 \\ b_1 \\ b_2 \end{Bmatrix}. \tag{1.52}$$

Consider approximation of the function $f(x) = e^x$. Since $e^0 = 1$ and $f^{(i)}(0) = e^0 = 1$, the equation systems to be solved are

$$\begin{bmatrix} 1/2 & 1 \\ 1/6 & 1/2 \end{bmatrix} \begin{Bmatrix} b_1 \\ b_2 \end{Bmatrix} = \begin{Bmatrix} -1/6 \\ -1/24 \end{Bmatrix} \tag{1.53}$$

and

$$\begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1/2 & 1 & 1 \end{bmatrix} \begin{Bmatrix} 1 \\ b_1 \\ b_2 \end{Bmatrix}. \tag{1.54}$$

Their solution is: $b_1 = -1/2$, $b_2 = 1/12$, $a_0 = 1$, $a_1 = 1/2$ and $a_2 = 1/12$. Therefore, the function $f(x) = e^x$ can be approximated with

$$R_{2,2}(x) = \frac{1 + x/2 + x^2/12}{1 - x/2 + x^2/12} \quad \text{or} \quad R_{2,2}(x) = \frac{12 + 6x + x^2}{12 - 6x + x^2}. \tag{1.55}$$

By using the same procedure other approximations of the function $f(x) = e^x$ can be found, such as

$$\begin{aligned} R_{4,0}(x) &= 1 + x + \tfrac{1}{2}x^2 + \tfrac{1}{6}x^3 + \tfrac{1}{24}x^4, \\ R_{3,1}(x) &= \frac{24 + 18x + 6x^2 + x^3}{24 - 6x}, \\ R_{1,3}(x) &= \frac{24 + 6x}{24 - 18x + 6x^2 - x^3}, \\ R_{0,4}(x) &= \frac{1}{1 - x + \tfrac{1}{2}x^2 - \tfrac{1}{6}x^3 + \tfrac{1}{24}x^4}. \end{aligned} \tag{1.56}$$

Note that $R_{4,0}(x)$ is equivalent to the polynomial obtained as Maclaurin series (1.33) truncated to the first five elements.

1.1.4 Comparison of approximation errors

In approximations by using Taylor or Maclaurin series expansion, as well as in Padé approximations, error increases rapidly away from the centre of approximation interval. This can be illustrated by Padé approximations of the function $f(x) = e^x$ at point $\xi = 0$ with the rational functions R_{nm} ($n + m = 2$), which are described in Example 1.5. The approximations based on Taylor and Maclaurin expansions are special cases of Padé approximations with polynomial $R_{n,0}$.

Comparison of approximation errors $E = e^x - R_{nm}(x)$ of the function $f(x) = e^x$ at point $\xi = 0$ is given in Tab. 1.1 and illustrated by plots in Fig. 1.1. Comparison of corresponding relative errors is given in Tab.1.2 and illustrated by plots in Fig. 1.2. Among the analysed approximations, the smallest relative approximation error $E/e^x = 1 - R_{nm}(x)/e^x$ on the interval $[-1,1]$ has Padé approximation with the rational function $R_{2,2}(x)$. In addition, the function $R_{2,2}(x)$ requires less numerical operations then the polynomial $R_{4,0}(x)$ that can be obtained by Maclaurin series expansion.

Tab. 1.1. Errors $E = e^x - R_{nm}(x)$ in Padé approximation of e^x at $\xi = 0$

x	e^x	(n,m)				
		(4,0)	(3,1)	(2,2)	(1,3)	(0,4)
–1	0,3679	–0,0071	0,0012	–0,00054	0,00053	–0,0014
–0,75	0,4724	–0,0018	0,00033	–0,00016	0,00018	–0,00050
–0,5	0,6065	–0,00024	0,000049	–0,000027	0,000032	–0,00010
–0,25	0,7788	–0,0000078	0,0000018	–0,0000011	0,0000014	–0,0000052
0	1	0	0	0	0	0
0,25	1,2840	0,0000086	–0,0000023	0,0000018	–0,0000029	0,000013
0,5	1,6487	0,00028	–0,000088	0,000073	–0,00013	0,00065
0,75	2,1170	0,0023	–0,00079	0,00072	–0,0015	0,0078
1	2,7183	0,010	–0,0039	0,0040	–0,0090	0,052

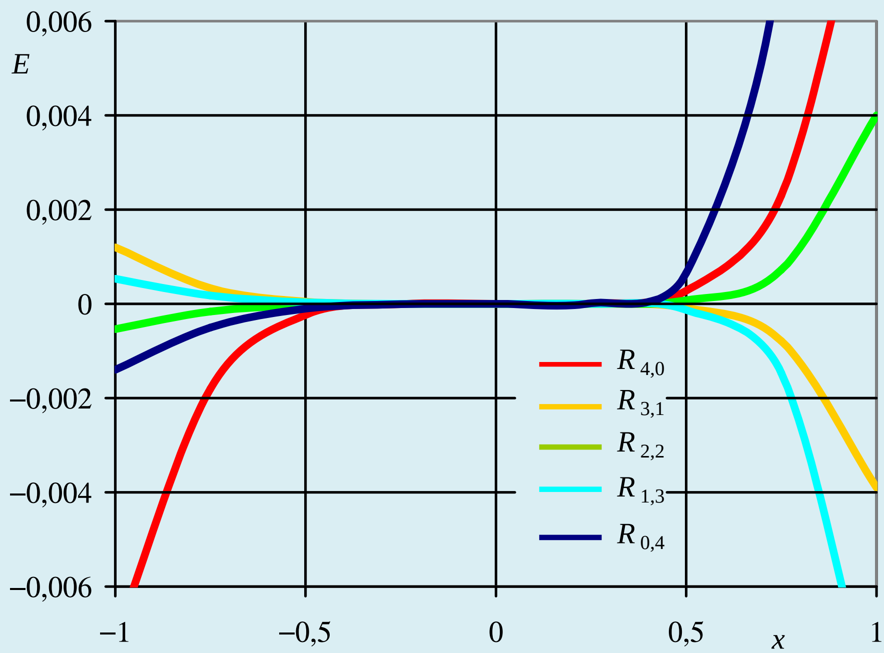

***Fig. 1.1.** Comparison of errors $E = e^x - R_{nm}(x)$ for Maclaurin ($R_{4,0}$) and Padé approximations of e^x at $\xi = 0$*

Tab. 1.2. Relative errors $1-R_{nm}(x)/e^x$ in Padé approximation of e^x at $\xi=0$

x	e^x	(n,m)				
		(4,0)	(3,1)	(2,2)	(1,3)	(0,4)
–1	0,3679	–0,019	0,0033	–0,0015	0,0014	–0,0037
–0,75	0,4724	–0,0038	0,00070	–0,00034	0,00037	–0,0011
–0,5	0,6065	–0,00040	0,000080	–0,000044	0,000053	–0,00017
–0,25	0,7788	–0,000010	0,0000023	–0,0000014	0,0000018	–0,0000010
0	1	0	0	0	0	0
0,25	1,2840	0,0000018	–0,0000018	0,0000014	–0,0000023	0,000010
0,5	1,6487	0,00017	–0,000053	0,000044	–0,000080	0,00040
0,75	2,1170	0,0011	–0,00037	0,00034	–0,00070	0,0038
1	2,7183	0,0037	–0,0014	0,0015	–0,0033	0,019

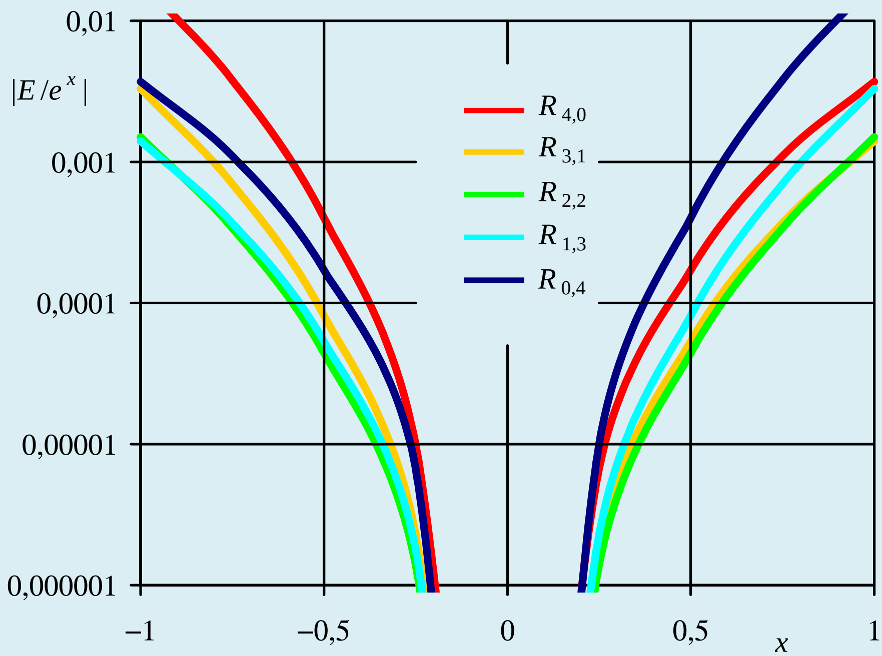

Fig. 1.2. *Comparison of relative errors* $|E/e^x|=|1-R_{mn}(x)/e^x|$ *for Maclaurin* ($R_{4,0}$) *and Padé approximations of* e^x *at* $\xi=0$

1.2 ORTHOGONAL SERIES EXPANSION

Consider an expansion of a function

$$f(x) = \sum_{n=0}^{\infty} \beta_n \phi_n(x), \quad x \in \Omega, \tag{1.57}$$

in a series of coordinate functions $\phi_n(x)$, which are orthogonal with respect to the so called *weighting function* $w(x)$ on a domain Ω. Such series, called *orthogonal series*, are generalisation of the *Fourier series* (Chapter 3).

1.2.1 Orthogonal functions on a continuous domain

Two functions $\phi_n(x)$ and $\phi_m(x)$ selected from a set of functions $\{\phi_n(x)\}$ are *orthogonal* with respect to a *weighting function* $w(x)$ on a continuous domain Ω (can be an interval, area, volume, etc.) if

$$\int_{\Omega} w(x)\phi_n(x)\phi_m(x)\,\mathrm{d}\Omega(x) \begin{cases} = 0, & n \neq m, \\ \neq 0, & n = m. \end{cases} \tag{1.58}$$

This integral is called *weighted inner product*. By introducing the following notation for the weighted inner product on a continuous domain[4]

$$\langle \phi, \psi \rangle = \int_{\Omega} w(x)\,\phi(x)\,\psi(x)\,\mathrm{d}\Omega(x)\,, \tag{1.59}$$

the condition of orthogonality (1.58) can be written in a simpler form

$$\langle \phi_m, \phi_n \rangle \begin{cases} = 0, & n \neq m, \\ \neq 0, & n = m. \end{cases} \tag{1.60}$$

If this relationship holds for all *m* and *n*, a family of functions $\phi_n(x)$ constitutes a *set of orthogonal functions* $\{\phi_n(x)\}$. Well known families of orthogonal functions are the sets $\{\sin n\varphi\}$ and $\{\cos n\varphi\}$ which are orthogonal on the interval $[-\pi, \pi]$. Several families of well-known polynomials do possess the property of orthogonality. The most known sets of such kind are the *Legendre*,

[4] Notation $\langle \phi, \psi \rangle$ for the weighted inner product is used instead of the form (ϕ, ψ) frequently used in some mathematical books, to avoid confusion in interpretation of terms $\tilde{f}(x, \beta)$, $x(x_1, x_2)$, etc.

Chebyshev, *Laguerre* and *Hermite polynomials*. The set of *monomials*[5] such as 1, x, x^2, x^3, ... , x^n (superscripts are exponents) are not orthogonal.

The special class of orthogonal functions are *orthonormal functions*. If a weighting function $w(x)$ is positive on a domain Ω, possibly with a finite number of zeros, than the inner product

$$\langle \phi_n, \phi_n \rangle = \int_\Omega w(x)\,[\phi_n(x)]^2 \,\mathrm{d}\Omega(x) \tag{1.61}$$

is positive and a set of orthogonal functions $\{\phi_n(x)\}$ can be *normalised* by dividing each function $\phi_n(x)$ with its *norm*[6] [3]

$$\|\phi_n\| = \sqrt{\langle \phi_n, \phi_n \rangle}\,. \tag{1.62}$$

The *normalised* set of functions

$$\bar{\phi}_n(x) = \frac{\phi_n(x)}{\|\phi_n\|} \quad \text{(for each } n\text{)}, \tag{1.63}$$

is said to be *orthonormal* with respect to a weighting function $w(x)$ on a domain Ω. These functions have the property

$$\langle \bar{\phi}_m, \bar{\phi}_n \rangle = \begin{cases} 0, & n \neq m, \\ 1, & n = m, \end{cases} \tag{1.64}$$

or, shorter

$$\langle \bar{\phi}_m, \bar{\phi}_n \rangle = \delta_{mn}\,. \tag{1.65}$$

Herein, δ_{mn} represents the Kronecker's delta symbol that has values $\delta_{mn} = 1$ for $m = n$ and $\delta_{mn} = 0$ for $m \neq n$.

---

[5] Monomial is any value obtained from 1 by finitely many multiplications by a variable or variables. If only a single variable *x* is considered this means that any monomial is either 1 or a power x^n of *x*, with *n* as positive integer. If several variables are considered, say, x_1, x_2 and x_3, then each can be given an exponent, so that any monomial is of the form $x_1^{n_1} x_2^{n_2} x_3^{n_3}$ with n_1, n_2 and n_3 a nonnegative integers (taking note that any exponent 0 makes the corresponding factor equal to 1). Notation can be shortened by writing $n = (n_1, n_2, n_3)$, when it can be defined $x^n = x_1^{n_1} x_2^{n_2} x_3^{n_3}$.

[6] In general, the *p*-norm is defined as $\|\phi_n\|_p = \sqrt[p]{\int_\Omega w(x)\,[\phi_n(x)]^p \,\mathrm{d}\Omega(x)}$.

1.2.2 Orthogonal functions on a discrete domain

Two functions $\phi_n(x)$ and $\phi_m(x)$ selected from a family of functions $\{\phi_n(x)\}$ are *orthogonal* with respect to *weighting coefficients* w^k over a discrete domain (i.e. a finite set of *K* distinct points ξ^k) if

$$\sum_{k=1}^{K} w^k \phi_n(\xi^k)\,\phi_m(\xi^k) \begin{cases} = 0, & n \neq m, \\ \neq 0, & n = m. \end{cases} \tag{1.66}$$

The sum on the left side is called *weighted inner product*, as the integral on a continuous domain (1.58). By introducing the following notation for the weighted inner product on a discrete domain

$$\langle \phi, \psi \rangle = \sum_{k=1}^{K} w^k \phi(\xi^k)\,\psi(\xi^k)\,, \tag{1.67}$$

the condition of orthogonality (1.66) can be written in a simpler form which is equal to that in the continuous case (1.60). The difference is only in the definitions of inner products (1.59) and (1.67).

If condition (1.66) holds for all *m* and *n*, the family of functions $\{\phi_n(x)\}$ constitutes a *set of orthogonal functions on a discrete domain*. Well known families of orthogonal functions on a discrete domain are the sets $\{\sin n\varphi\}$ and $\{\cos n\varphi\}$ which are orthogonal on the equidistant set of points on the interval $[-\pi, \pi]$. Several families of well-known polynomials do also possess a property of orthogonality on a discrete domain. The most known sets of such kind are the *Gram* and *Chebyshev polynomials*.

The special class of functions which are orthogonal on a discrete domain are *orthonormal functions*. If weighting coefficients w^k are positive, then the inner product on a discrete domain

$$\langle \phi_n, \phi_n \rangle = \sum_{k=1}^{K} w^k [\phi_n(\xi^k)]^2 \tag{1.68}$$

is positive and a set of orthogonal functions $\phi_n(x)$ can be *normalised* by dividing each function $\phi_n(x)$ with its *norm* $\|\phi_n\| = \sqrt{\langle \phi_n, \phi_n \rangle}$.

Normalised functions $\bar{\phi}_n(x) = \phi_n(x)/\|\phi_n\|$ (for each n) are *orthonormal* with respect to weighting coefficients w^k on a particular finite set of K distinct points ξ^k. The properties of orthonormal functions are already specified by expression (1.64) (and (1.65)).

1.2.3 Expansion in orthogonal series (generalised Fourier coefficients)

Assuming that a series on the right side of equation (1.57) converges to $f(x)$ on a domain Ω, both sides of (1.57) can be multiplied by $w(x)\,\phi_m(x)$ and integrated over a domain Ω:

$$\int_\Omega w(x)\; f(x)\,\phi_m(x)\,\mathrm{d}\Omega = \sum_{n=0}^{\infty} \beta_n \int_\Omega w(x)\,\phi_n(x)\,\phi_m(x)\,\mathrm{d}\Omega\,. \tag{1.69}$$

Since the set of functions $\{\phi_m\}$ is considered orthogonal on a domain Ω, some integrals vanish. Therefore, it follows

$$\beta_n = \frac{\langle f, \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} = \frac{\int_\Omega w(x)\; f(x)\,\phi_n(x)\,\mathrm{d}\Omega}{\int_\Omega w(x)\,[\phi_n(x)]^2\,\mathrm{d}\Omega}\,. \tag{1.70}$$

So obtained coefficients β_n are called *generalised Fourier coefficients.*

Function $f(x)$ that depends on M arguments $x_1, x_2, ... x_M$ can be easily expanded into a series

$$f(x) = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} ... \sum_{n_M=0}^{\infty} \beta_{n_1 n_2 ... n_M}\, \phi_{n_1}^{[1]}(x_1)\phi_{n_2}^{[2]}(x_2)...\phi_{n_M}^{[M]}(x_M) \tag{1.71}$$

of functions $\phi_{n_1}^{[1]}$, $\phi_{n_2}^{[2]}$, …, $\phi_{n_M}^{[M]}$ that are orthogonal with respect to functions $w^{[1]}(x_1), w^{[2]}(x_2), ..., w^{[M]}(x_M)$ on independent intervals $[a_1, b_1]$, $[a_2, b_2]$, …, $[a_M, b_M]$ (Fig. 1.3), i.e. into a series of coordinate functions that satisfy condition

$$(\forall r = 1, 2, ..., M)$$
$$\int_{a_r}^{b_r} w^{[r]}(x_r)\phi_{n_r}^{[r]}(x_r)\phi_{m_r}^{[r]}(x_r)\,\mathrm{d}x_r \begin{cases} = 0, & m_r \neq n_r, \\ \neq 0, & m_r = n_r. \end{cases} \tag{1.72}$$

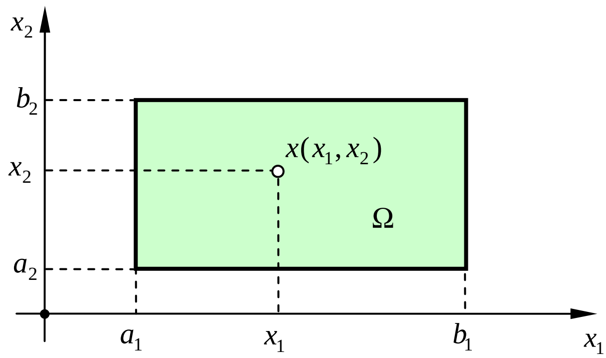

Fig. 1.3. *Example of independent intervals in the 2D space*

Both sides of the series (1.71) can be multiplied by $\phi_{m_1}^{[1]}(x_1)\phi_{m_2}^{[2]}(x_2)...\phi_{m_M}^{[M]}(x_M)$ and $w(x) = w^{[1]}(x_1)w^{[2]}(x_2)...w^{[M]}(x_M)$, and integrated over intervals $[a_1, b_1]$, $[a_2, b_2]$, …, $[a_M, b_M]$. The results are generalised Fourier coefficients

$$\beta_{n_1 n_2 ... n_M} = \frac{\int_{a_1}^{b_1}\int_{a_2}^{b_2}...\int_{a_M}^{b_M} w(x) f(x) \phi_{n_1}^{[1]}(x_1)\phi_{n_2}^{[2]}(x_2)...\phi_{n_M}^{[M]}(x_M) \mathrm{d}x_1 \mathrm{d}x_2 ... \mathrm{d}x_M}{\left(\int_{a_1}^{b_1} w^{[1]}(x_1)[\phi_{n_1}^{[1]}(x_1)]^2 \,\mathrm{d}x_1\right)...\left(\int_{a_M}^{b_M} w^{[M]}(x_M)[\phi_{n_M}^{[M]}(x_M)]^2 \,\mathrm{d}x_M\right)}. \quad (1.73)$$

Approximation function $\tilde{f}(x, \beta)$ (1.4) (or (1.6)) is a partial sum of the first N (or $N = N_1 N_2 \dots N_M$) elements.

It should be emphasized that once when an approximation of a function $f(x)$ by using generalised Fourier coefficients β_n is found, it is not necessary to recompute these coefficients when the number of elements in a partial sum S_N (1.10) is changed (e.g. for finding a better approximation by including more elements of series in summation). This is sometimes referred to as the *principle of finality*.

1.2.4 Approximation on a discrete domain

Consider that an approximated function $f(x)$ is defined by a table, i.e. by sampling values $f^k = f(\xi^k)$ in a finite set of K sampling points ξ^k. Generalised Fourier coefficients are [4]:

$$\beta_n = \frac{\langle f, \phi_n \rangle}{\langle \phi_n, \phi_n \rangle} = \frac{\sum_{k=1}^{K} w^k f^k \phi_n(\xi^k)}{\sum_{k=1}^{K} w^k [\phi_n(\xi^k)]^2}. \tag{1.74}$$

Although approximation function $\tilde{f}(x,\beta)$ in the discrete case has the form equal to that in the continuous case (1.10), there is one crucial difference. By the K values $f^k = f(\xi^k)$ of function $f(x)$ in the K distinct sampling points ξ^k it can be determined up to K generalised Fourier coefficients β_n ($n = 0, 1, ..., K-1$). Coefficients β_n ($n \geq K$) are assumed to be zero.

Therefore, an approximation function $\tilde{f}(x,\beta)$ is restricted to the first K summands $\beta_n \phi_n$ (i.e. $n = 0, 1, ..., N-1$ and $N \leq K$). Using all N summands $\beta_n \phi_n$ turns the approximation into the *interpolation* (i.e. in that case $\tilde{f}(\xi^k, \beta) = f^k$ for all sampling points ξ^k).

In the case when a function $f(x)$ depends on M arguments $x_1, x_2, ... x_M$, sampling points can be arranged in the form of mesh, as those shown in Fig. 1.4.

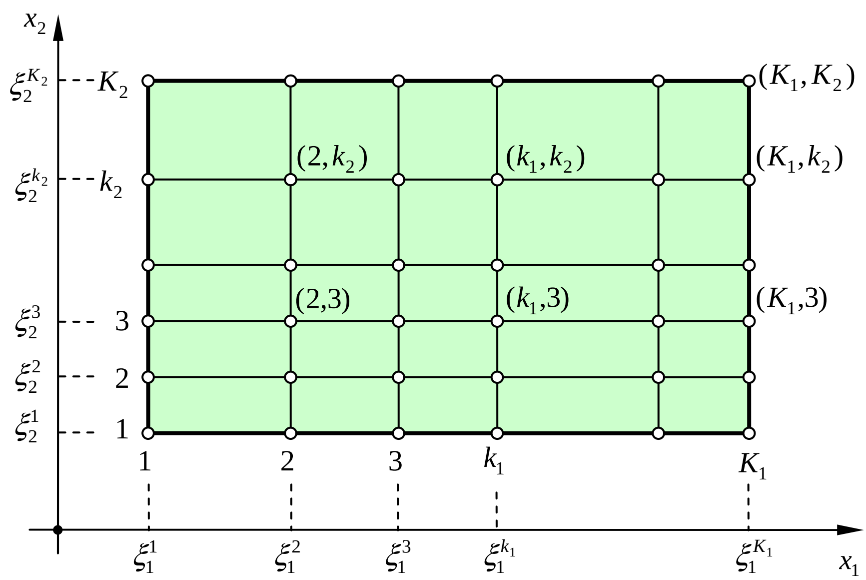

Fig. 1.4. *Example of a mesh of sampling points in the 2D space*

In this case, a function $f(x)$ can be easily approximated with the series (1.71) of coordinate functions $\phi_{n_r}^{[r]}(x_r)$ that can be grouped into the sets $\{\phi_{n_1}^{[1]}(x_1)\}$, $\{\phi_{n_2}^{[2]}(x_2)\}$, …, $\{\phi_{n_M}^{[M]}(x_M)\}$. Each set of these functions $\phi_{n_r}^{[r]}(x_r)$ (for particular r) are orthogonal with respect to the corresponding set of coefficients $\{w^{k_r[r]}\} = \{w^{1[r]}, w^{2[r]}, ..., w^{K_r[r]}\}$, i.e. it is assumed that all sets of these coordinate functions satisfy the condition of orthogonality

$$(\forall r = 1, 2, ..., M)$$

$$\sum_{k_r=1}^{K_r} w^{k_r[r]}\, \phi_{n_r}^{[r]}(\xi_r^{k_r})\, \phi_{m_r}^{[r]}(\xi_r^{k_r}) \begin{cases} = 0, & m_r \neq n_r, \\ \neq 0, & m_r = n_r. \end{cases} \tag{1.75}$$

Both sides of the series (1.71) can be multiplied by $w^{k_1[1]}\phi_{m_1}^{[1]}(\xi_1^{k_1})$, $w^{k_1[1]}\phi_{m_1}^{[1]}(\xi_1^{k_1})$, …, $w^{k_M[M]}\phi_{m_M}^{[M]}(\xi_M^{k_M})$ and summed over indexes $k_1 = 1, 2, ..., K_1$; $k_2 = 1, 2, ..., K_2$; …; $k_M = 1, 2, ..., K_M$. The result is a set of generalised Fourier coefficients

$$\beta_{n_1 n_2 \ldots n_M} = \frac{\sum_{k_1=1}^{K_1}\sum_{k_2=1}^{K_2}\cdots\sum_{k_M=1}^{K_M} w^{k_1 k_2 \ldots k_M} f^{k_1 k_2 \ldots k_M} \phi_{n_1}^{[1]}(\xi_1^{k_1})\phi_{n_2}^{[2]}(\xi_2^{k_2})\ldots\phi_{n_M}^{[M]}(\xi_M^{k_M})}{\left(\sum_{k_1=1}^{K_1} w^{k_1[1]}[\phi_{n_1}^{[1]}(\xi_1^{k})]^2\right)\cdot\ldots\cdot\left(\sum_{k_M=1}^{K_M} w^{k_M[\mathrm{M}]}[\phi_{n_M}^{[M]}(\xi_M^{k_M})]^2\right)}, \tag{1.76}$$

where $w^{k_1 k_2 \ldots k_M} = w^{k_1[1]} w^{k_2[2]} \cdots w^{k_M[M]}$. Only the first $K = K_1 K_2 \cdots K_M$ coefficients can be determined. Therefore, the approximation function $\tilde{f}(x, \beta)$ is restricted to the first K summands.

1.2.5 Convergence of orthogonal series

Orthogonal series (1.57) with generalised Fourier coefficients β_n (1.70) or (1.74) corresponds to the function $f(x)$. But, it is a priori unknown if a partial sum S_N (1.10) converges or even, when it does converge, does it converge to $f(x)$. In practice, convergence is assured if $f(x)$ and its first derivative $f'(x)$ are piecewise continuous on a domain Ω.

A function $f(x)$ is said to be *piecewise continuous* on a domain if

(i) the domain can be divided into a finite number of subdomains in each of which $f(x)$ is continuous and

(ii) the limits of $f(x)$ as x approaches boundary of each subdomain are finite.

Example of the piecewise continuous function $f(x)$ defined on an interval $[a,b]$ is shown on Fig. 1.5. On each subinterval the function $f(x)$ is continuous and the limits of the function $f(x)$ as x approaches endpoints of each subinterval are finite.

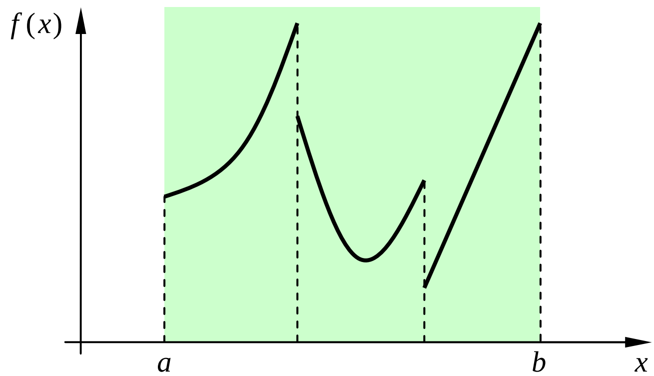

Fig. 1.5. *Example of piecewise continuous function on* $[a,b]$

In other words, piecewise continuous function is the one that has at most a finite number of finite discontinuities [5].

1.3 LEAST-SQUARES APPROXIMATION

The principles of least-squares[7] is in minimising the integral of the squared approximation error $[f(x)-\tilde{f}(x,\beta)]^2$ (optionally multiplied by *weighting function*) over a given domain (in the approximation of continuous type), or in minimising the sum of the squared approximation error $[f(\xi^k)-\tilde{f}(\xi^k,\beta)]^2$ (optionally multiplied by *weighting coefficients*) over a discrete set of K distinct points ξ^k (in the approximation of discrete type).

[7] The principles of least-squares are independently discovered by German Carl Fridrich Gauss (1795), Frenchman Adrien-Marie Legendre (1805) and American Robert Adrian (1808). An early demonstration of the strength of the method came when it was used to predict the future position of the newly discovered asteroid Ceres in 1981. On January 1, 1981, the Italian astronomer Giuseppe Piazzi discovered Ceres and was able to track its path 40 days before it was lost in the glare of the sun. The only predictions that successfully allowed Hungarian astronomer Franz Xaver von Zach to relocate the Ceres where those performed by the Gauss using least-squares analysis.

In a general case, a function

$$g(x) = \sqrt{w(x)}\ f(x) \tag{1.77}$$

is approximated by an approximation function

$$\tilde{g}(x, \beta_k) = \sqrt{w(x)}\ \tilde{f}(x, \beta_k)\,, \tag{1.78}$$

where $w(x)$ is a positive function (in trivial case $w(x) = 1$) applied “as is” (without approximation). A function $f(x)$ is approximated with an approximation function $\tilde{f}(x, \beta)$.

1.3.1 Least-squares on a continuous domain

Approximation error is defined as

$$g(x) - \tilde{g}(x, \beta) = \sqrt{w(x)}\,[f(x) - \tilde{f}(x, \beta)] = \sqrt{w(x)}\ R(x, \beta)\,. \tag{1.79}$$

If the functions $g(x)$ and $f(x)$ depend on the single argument *x*, the mean square error is defined on an interval $[a, b]$ by

$$\begin{aligned} E_{\text{ms}}(\beta) &= \frac{1}{b-a}\int_a^b w(x) R^2(x, \beta)\,\mathrm{d}x \\ &= \frac{1}{b-a}\int_a^b w(x)[f(x) - \tilde{f}(x, \beta)]^2\,\mathrm{d}x. \end{aligned} \tag{1.80}$$

In the general case functions $g(x)$, $f(x)$, … can depend on *M* coordinates $x_1, x_2, \ldots x_M$ of a point $x = x(x_1, x_2, \ldots, x_M)$. For that reason it is convenient to define the mean square error on a domain Ω (can be an interval, area, volume, etc.) as

$$\begin{aligned} E_{\text{ms}}(\beta) &= \frac{1}{\int_\Omega \mathrm{d}\Omega(x)}\int_\Omega w(x) R^2(x, \beta)\,\mathrm{d}\Omega(x) \\ &= \frac{1}{\int_\Omega \mathrm{d}\Omega(x)}\int_\Omega w(x)[f(x) - \tilde{f}(x, \beta)]^2\,\mathrm{d}\Omega(x)\,. \end{aligned} \tag{1.81}$$

The *least-squares method* consists in minimising the mean square error $E_{\text{ms}}(\beta)$ on a given domain Ω by choosing adequate coefficients β_n. From the condition of extreme in the respect to the coefficients β_n it follows

$$\frac{\partial E_{\mathrm{ms}}(\beta)}{\partial \beta_m} = 0 \Rightarrow \int_{\Omega} w(x)[f(x) - \tilde{f}(x,\beta)] \frac{\partial \tilde{f}(x,\beta)}{\partial \beta_m} \mathrm{d}\Omega(x) = 0 . \qquad (1.82)$$

For an approximation function of linear type $\tilde{f}(x,\beta) = \sum_n \beta_n \phi_n(x)$ and its derivative

$$\frac{\partial \tilde{f}(x,\beta)}{\partial \beta_m} = \sum_{n=0}^{N-1} \frac{\partial \beta_n}{\partial \beta_m} \phi_n(x) = \phi_m(x) , \qquad (1.83)$$

it follows

$$(\forall m = 0, ..., N-1)$$
$$\int_{\Omega} w(x) f(x) \phi_m(x) \mathrm{d}\Omega(x) - \sum_{n=0}^{N-1} \beta_n \int_{\Omega} w(x) \phi_n(x) \phi_m(x) \mathrm{d}\Omega(x) = 0. \qquad (1.84)$$

This linear equation system can be expressed in the terms of weighted inner product on a continuous domain (1.59) as

$$(\forall m = 0, ..., N-1) \quad \sum_{n=0}^{N-1} \langle \phi_n, \phi_m \rangle \beta_n = \langle f, \phi_m \rangle . \qquad (1.85)$$

Therefore, unknown coefficients β_n can be found by solving linear equation system

$$(\forall m = 0, ..., N-1) \quad \sum_{n=0}^{N-1} a_{mn} \beta_n = b_m \qquad (1.86)$$

determined with coefficients

$$a_{mn} = \langle \phi_n, \phi_m \rangle = \int_{\Omega} w(x)\, \phi_n(x)\, \phi_m(x)\, \mathrm{d}\Omega ,$$
$$b_m = \langle f, \phi_m \rangle = \int_{\Omega} w(x)\; f(x)\, \phi_m(x)\, \mathrm{d}\Omega(x) . \qquad (1.87)$$

Unfortunately, the linear equation system obtained by the least-squares method can be *ill-conditioned* so that its numerical solution (coefficients β_n) can have intolerable error (see example at the end of Chapter 1.3.2).

1.3.2 Least-squares on a discrete domain

Let the approximated function $f(x)$ be defined by a table, i.e. by sampling values $f^k = f(\xi^k)$ on the finite set of K sampling points ξ^k. The mean square error is defined as a sum of weighted squared residuals on K sampling points ξ^k :

$$\begin{aligned} E_{\mathrm{ms}}(\beta) &= \frac{1}{K}\sum_{k=1}^{K} w^k R^2(\xi^k,\beta) \\ &= \frac{1}{K}\sum_{k=1}^{K} w^k [f^k - \tilde{f}(\xi^k,\beta)]^2. \end{aligned} \tag{1.88}$$

Weighting coefficients w^k are considered positive.

From the condition of extreme in the respect to coefficients β_m

$$(\forall m < K) \quad \frac{\partial E_{\mathrm{ms}}(\beta)}{\partial \beta_m} = 0\,, \tag{1.89}$$

it follows

$$\sum_{k=1}^{K} w^k [f^k - \tilde{f}(\xi^k,\beta)] \frac{\partial \tilde{f}(\xi^k,\beta)}{\partial \beta_m} = 0\,. \tag{1.90}$$

In the approximation of linear type, derivative of approximation function $\tilde{f}(\xi^k,\beta)$ (1.4) at the point ξ^k is

$$\frac{\partial \tilde{f}(\xi^k,\beta)}{\partial \beta_m} = \sum_{n=0}^{N-1} \frac{\partial \beta_n}{\partial \beta_m} \phi_n(\xi^k) = \phi_m(\xi^k)\,. \tag{1.91}$$

Substitution of this derivative into (1.90) gives linear equation system

$$\begin{aligned} &(\forall m = 0,1,\ldots,N-1) \\ &\qquad \sum_{k=1}^{K} w^k f^k \phi_m(\xi^k) - \sum_{n=0}^{N-1} \beta_n \sum_{k=1}^{K} w^k \phi_n(\xi^k)\, \phi_m(\xi^k) = 0, \end{aligned} \tag{1.92}$$

whose solution are coefficients β_n ($n = 0,1,\ldots,N-1$, where $N \le K$).

This linear equation system can be expressed in the terms of the weighted inner product (1.67) on a discrete domain as

$$(\forall m = 0,1,\ldots,N-1) \quad \sum_{n=0}^{N-1} \langle \phi_n, \phi_m \rangle \beta_n = \langle f, \phi_m \rangle, \quad N \le K\,. \tag{1.93}$$

This linear equation system is the same as that obtained by the least-squares method on a continuous domain, but limited to $N \le K$ equations. Therefore, the unknown coefficients β_n can be found by solving linear equation system

$$(\forall m = 0,\ldots,N-1) \quad \sum_{n=0}^{N-1} a_{mn} \beta_n = b_m\,, \quad N \le K\,, \tag{1.94}$$

determined with coefficients

$$a_{mn} = \langle \phi_n, \phi_m \rangle = \sum_{k=1}^{K} w^k \phi_n(\xi^k)\, \phi_m(\xi^k),$$
$$b_m = \langle f, \phi_m \rangle = \sum_{k=1}^{K} w^k f^k \phi_m(\xi^k)\,. \tag{1.95}$$

As in approximation on a continuous domain, coefficients β_n found as a solution of linear equation system (1.94) can have intolerable error. Clearly, for the small values of *N*, say up to 6 or 7, experience indicates that a solution of (1.94) produces quite good least-squares approximation. But for the greater values of *N*, a solution found by solving (1.94) generally leads to the progressively poorer least-squares approximations [6]. An explanation of this can be found in the following example.

Example 1.6. Ill-conditioned matrix in the least-squares approximation. Substitution of $\phi_n(x) = x^n$ and $w^k = 1$ into (1.95) gives $a_{mn} = \sum_{k=1}^{K} (\xi^k)^{n+m}$. For convenience, it can be assumed that sampling points ξ^k are all distributed uniformly on the interval $[0,1]$. For a large number of sampling points *K* the approximation

$$a_{mn} = \sum_{k=1}^{K} (\xi^k)^{n+m} \approx \frac{K}{m+n+1}, \quad m,n = 0,\ldots, N-1, \tag{1.96}$$

should be a good one. Let $\mathbf{A} = [a_{mn}]$ be a matrix of coefficients in (1.94) that can be approximated with *K* times the matrix $\mathbf{H}_N$, where

$$\mathbf{H}_N = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \ldots & \frac{1}{N} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \ldots & \frac{1}{N+1} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \ldots & \frac{1}{N+2} \\ \ldots & \ldots & \ldots & & \ldots \\ \frac{1}{N} & \frac{1}{N+1} & \frac{1}{N+2} & \ldots & \frac{1}{2N-1} \end{bmatrix}. \tag{1.97}$$

This matrix is the principal minor of order *N* of the so called infinite *Hilbert matrix* and represents classical example of an *ill-conditioned matrix.*

A matrix is ill-conditioned if, when it has been normalised so that its largest element has order of magnitude 1 (as element in the first row and column of matrix $\mathbf{H}_N$), its inverse has very large elements. For example, when $N = 6$, the inverse of $\mathbf{H}_6$ has elements of magnitude $4 \cdot 10^6$ [7]: (1.98)

$$\mathbf{H}_6^{-1} = \begin{bmatrix} 36 & & & & & \\ -630 & 14700 & & & \textit{symmetric} & \\ 3360 & -88200 & 564480 & & & \\ -7360 & 211680 & -1411200 & 3628800 & & \\ 7560 & -220500 & 1512000 & -3969000 & 4410000 & \\ -2772 & 83160 & -582120 & 1552320 & -1746360 & 698544 \end{bmatrix}.$$

When $N = 10$, the inverse of $\mathbf{H}_{10}$ has elements of magnitude $3 \cdot 10^{12}$. The result of this is that any round-off error incurred in entering the coefficients of $\mathbf{H}_N$ into the computer would result in an inverse matrix whose huge coefficients greatly magnify initial round-off errors making the final result useless.

1.3.3 Least-squares with orthogonal functions

Solving linear equation system (1.86) or (1.94) obtained by least-squares, can be avoided if the chosen family of functions $\{\phi_n(x)\}$ constitutes a set of orthogonal functions (Chapter 1.2).

By using an orthogonal set of functions ϕ_n, i.e. the functions that satisfy the condition of orthogonality (1.58) or (1.66), the coefficients a_{mn} in (1.87) or (1.95) in linear equation system (1.86) or (1.94) obtained by the least-squares become

$$a_{mn} = \langle \phi_m, \phi_n \rangle = \begin{cases} 0, & m \neq n, \\ \langle \phi_n, \phi_n \rangle, & m = n. \end{cases} \tag{1.99}$$

The solution of linear equation system (1.86) or (1.94), the coefficients β_n, become equal to generalised Fourier coefficients $\beta_n = \langle f, \phi_n \rangle / \langle \phi_n, \phi_n \rangle$ (1.70) or (1.74) that have already been obtained by the orthogonal series expansion. Therefore, they are independent of a number of equations.

For that reason, it is often said that approximation function $\tilde{f}(x, \beta)$ (1.4) as a partial sum $S_N(x, \beta)$ (1.10) of the first N elements of orthogonal series, in which β_n are generalised Fourier coefficients, is an *approximation* in the *least-square sense* or a *least-square approximation* of a function $f(x)$.

2. LEAST-SQUARES POLYNOMIAL APPROXIMATION

Due to its simplicity, a least-squares polynomial approximation is the most frequently used type of the least-squares approximations. It can be applied on a continuous domain and on a discrete domain.

2.1 APPROXIMATION ON A CONTINUOUS DOMAIN

Let the function $f(x)$ be approximated with the polynomial

$$\tilde{f}(x,\alpha) = \sum_{r=0}^{N-1} \alpha_r x^r \;, \tag{2.1}$$

whose coefficients α_r are determined by the least-squares method, as it is described in this chapter.

By analogy to (1.80), the mean square error is defined on an interval $[a,b]$ as

$$\begin{aligned} E_{\mathrm{ms}}(\alpha) &= \frac{1}{b-a}\int_a^b w(x)[f(x)-\tilde{f}(x,\alpha)]^2 \,\mathrm{d}x \\ &= \frac{1}{b-a}\int_a^b w(x)\left(f(x)-\sum_{r=0}^{N-1}\alpha_r x^r \right)^2 \mathrm{d}x \,. \end{aligned} \tag{2.2}$$

From the condition of extreme in the respect to coefficients α_r it follows

$$(\forall n = 0, ..., N-1) \quad \frac{\partial E_{\mathrm{ms}}(\alpha)}{\partial \alpha_n} = 0 \Rightarrow \int_a^b w(x) \left(f(x) - \sum_{r=0}^{N-1} \alpha_r x^r \right) x^n \, \mathrm{d}x = 0, \tag{2.3}$$

or

$$(\forall n = 0, ..., N-1) \quad \sum_{r=0}^{N-1} \alpha_r \int_a^b w(x)\, x^{r+n} \, \mathrm{d}x = \int_a^b w(x)\, f(x)\, x^n \, \mathrm{d}x . \tag{2.4}$$

This linear equation system can be expressed in the terms of weighted inner product on an interval $[a,b]$:

$$\langle \phi, \psi \rangle = \int_a^b w(x)\, \phi(x)\, \psi(x) \, \mathrm{d}x \tag{2.5}$$

as

$$(\forall n = 0, ..., N-1) \quad \sum_{r=0}^{N-1} \alpha_r \langle x^r, x^n \rangle = \langle f, x^n \rangle . \tag{2.6}$$

Solution of this linear equation system are coefficients α_r.

As it is already outlined in Chapter 1.3.1, a linear equation system obtained by the least-squares method can be ill-conditioned and its numerical solution (coefficients α_r) can have intolerable error.

To avoid solving the linear equation system (2.6), function $f(x)$ can be expanded into the series

$$f(x, \beta) = \sum_{n=0}^{\infty} \beta_n p_n(x) \tag{2.7}$$

of orthogonal polynomials

$$p_n(x) = \sum_{r=0}^{n} a_{nr} x^r = a_{nn} x^n + a_{n,n-1} x^{n-1} + ... + a_{n,1} x + a_{n,0} , \tag{2.8}$$

i.e., the polynomials whose coefficients a_{nr} are determined by the orthogonality condition

$$\langle p_n, p_m \rangle = \int_a^b w(x)\, p_n(x)\, p_m(x)\, \mathrm{d}x \begin{cases} = 0, & m \neq n, \\ \neq 0, & m = n, \end{cases} \tag{2.9}$$

with respect to some weighting function $w(x)$ on an interval $[a,b]$.

Orthogonal polynomials $p_n(x)$ are a very important subclass of orthogonal functions. They are defined to be such that the *n*-th polynomial is of degree exactly *n*, and they naturally have all the properties of orthogonal functions plus the peculiarity of polynomials.

The coefficients β_n in expansion (2.7) are generalised Fourier coefficients that can be obtained by setting $\phi_n(x) = p_n(x)$ into (1.70) as

$$\beta_n = \frac{\langle f, p_n \rangle}{\langle p_n, p_n \rangle} = \frac{\int_a^b w(x)\; f(x)\; p_n(x)\, \mathrm{d}x}{\int_a^b w(x)[\, p_n(x)]^2\, \mathrm{d}x}\,. \tag{2.10}$$

These coefficients can also be obtained by the least-squares method as it is described in Chapter 1.3. For that reason it is often said that the approximation function

$$\tilde{f}(x,\beta) = \sum_{n=0}^{N-1} \beta_n p_n(x)\,, \tag{2.11}$$

defined as a partial sum of the first N elements containing the orthogonal polynomials $p_n(x)$ with degree *n* up to $N-1$, is the *polynomial least-squares approximation* of function $f(x)$.

A special class of orthogonal polynomials are *orthonormal polynomials*. If the weighting function $w(x)$ is positive on an interval $[a,b]$, possibly with the finite number of zeros, than the weighted inner product

$$\langle p_n, p_n \rangle = \int_a^b w(x)\,[\, p_n(x)]^2\, \mathrm{d}x \tag{2.12}$$

is positive and a set of orthogonal polynomials $\{p_n(x)\}$ can be *normalised* by dividing each polynomial $p_n(x)$ with its *norm* [3]:

$$\|p_n\| = \sqrt{\langle p_n, p_n \rangle}\,. \tag{2.13}$$

The *normalised* polynomials

$$\overline{p}_n(x) = \frac{p_n(x)}{\|p_n\|} \quad \text{(for each } n\text{)}, \tag{2.14}$$

are said to be *orthonormal* with respect to a weighting function $w(x)$ on an interval $[a,b]$. These polynomials have the properties

$$\langle \overline{p}_m, \overline{p}_n \rangle = \delta_{mn}, \quad \|\overline{p}_n\| = \sqrt{\langle \overline{p}_n, \overline{p}_n \rangle} = 1, \tag{2.15}$$

where δ_{mn} represents the *Kronecker's delta symbol* that is already defined in Chapter 1.2.1.

Hence, if a function $f(x)$ is expanded into a series of orthonormal polynomials

$$f(x, \overline{\beta}) = \sum_{n=0}^{\infty} \overline{\beta}_n \overline{p}_n(x), \tag{2.16}$$

the corresponding generalised Fourier coefficients are

$$\overline{\beta}_n = \langle f, \overline{p}_n \rangle = \int_a^b w(x)\, f(x)\, \overline{p}_n(x)\, \mathrm{d}x. \tag{2.17}$$

Form of approximation function $\tilde{f}(x,\beta)$ (2.11) is not convenient for numerical manipulation. By substituting orthogonal polynomials $p_n(x)$ (2.8) in approximation function $\tilde{f}(x,\beta)$ (2.11), it can be obtained

$$\tilde{f}(x,\beta) = \sum_{n=0}^{N-1} \left(\beta_n \sum_{r=0}^{n} a_{nr} x^r \right) = \sum_{r=0}^{N-1} \left(\sum_{n=r}^{N-1} \beta_n a_{nr} \right) x^r = \sum_{r=0}^{N-1} \alpha_r x^r. \tag{2.18}$$

Therefore, the approximation function $\tilde{f}(x,\beta)$ is polynomial of degree $N-1$ that can also be expressed in the form of $\tilde{f}(x,\alpha)$ (2.1). Coefficients α_r can be calculated from coefficients a_{nr} and β_n as

$$\alpha_r = \sum_{n=r}^{N-1} \beta_n a_{nr}. \tag{2.19}$$

They can be determined once for ever for the particular functions $f(x)$ and $w(x)$ defined on an interval $[a,b]$ whose boundaries can be finite or infinite.

2.2 ORTHOGONAL POLYNOMIALS ON A CONTINUOUS DOMAIN

There are several polynomial family sets orthogonal with respect to different weighting functions $w(x)$ on a continuous interval, some of which are listed in Tab. 2.1. The most important are *Legendre polynomials*, *Chebyshev polynomials*, *Jacobi polynomials*, *Laguerre polynomials* and *Hermite polynomials*.

Tab. 2.1. Classical orthogonal polynomials on a continuous domain

Name	Symbol	Domain	Weighting function	Chapter
Legendre	$P_n(x)$	$[-1,1]$	1	2.2.3
Associated Legendre	$P_n^k(x)$	$[-1,1]$	1	2.2.4
Shifted Legendre	$P_n^*(x)$	$[0,1]$	1	2.2.6
Chebyshev (1st kind)	$T_n(x)$	$[-1,1]$	$1/\sqrt{1-x^2}$	4.1
Chebishev, shifted	$T_n^*(x)$	$[0,1]$	$1/\sqrt{x-x^2}$	4.2
Chebishev, 2nd kind	$U_n(x)$	$[-1,1]$	$\sqrt{1-x^2}$	4.4
Jacobi	$Q_n^{\alpha\beta}(x)$	$[-1,1]$	$(1-x)^\alpha(1+x)^\beta$, $\alpha,\beta>-1$	2.2.9
Ultraspherical or Gegenbauer	$C_n^\alpha(x)$	$[-1,1]$	$(1-x^2)^{\alpha-1/2}$, $\alpha>-1/2$	2.2.9
Laguerre	$L_n(x)$	$[0,\infty)$	e^{-x}	2.2.10
Laguerre, generalized	$L_n^\alpha(x)$	$[0,\infty)$	$x^\alpha e^{-x}$, $\alpha>-1$	2.2.11
Hermite, probabilists'	$H_n(x)$	$(-\infty,\infty)$	$e^{-x^2/2}$	2.2.12
Hermite, phisicists'	$H_n(x)$	$(-\infty,\infty)$	e^{-x^2}	2.2.12
Zernike	$Z_n^{\pm m}(\rho,\varphi)$	Unit disc	$\rho=\sqrt{x_1{}^2+x_2{}^2}$	2.3.1

It is also possible to find a set of polynomials that are orthogonal with respect to an arbitrary weighting function $w(x)$ on an arbitrary interval $[a,b]$. Due to its importance, some polynomials and related algorithms are described in the following chapters, as it is listed in Table 2.1. In addition, in Chapters 2.2.1 and 2.2.2 two general algorithms are presented for generating polynomials orthogonal with respect to an arbitrary weighting function $w(x)$ on an arbitrary interval $[a,b]$. These two algorithms are based on different approaches, but they provide the same results.

2.2.1 Generating orthogonal polynomials

For any weighting function $w(x)$, which is positive everywhere (except possibly in a finite set of points ς^k where $w(\varsigma^k)=0$) and integralable on a closed interval $[a,b]$, there exists a corresponding set of orthogonal polynomials [7].

Let these orthogonal polynomials $p_n(x)$ be standardised so that their leading coefficients have value 1 (i.e., that they have the form $p_n(x)=x^n+...$). The monomial x^n of order n can be expanded with the first $n+1$ orthogonal polynomials $p_0(x), p_1(x), ..., p_n(x)$ by using the equation

$$x^n = p_n(x)+\sum_{m=0}^{n-1}\gamma_{nm}p_m(x)\,. \tag{2.20}$$

Therefore, the orthogonal polynomial $p_n(x)=x^n+...$, can be defined as

$$p_n(x)=x^n-\sum_{m=0}^{n-1}\gamma_{nm}p_m(x),\quad n\geq 1\,. \tag{2.21}$$

To find coefficients γ_{nm}, both sides of that equation can be multiplied by $w(x)p_r(x)$ and integrated over an interval $[a,b]$:

$$\begin{aligned}\int_a^b w(x)\,p_r(x)\,p_n(x)\,\mathrm{d}x &= \\ &=\int_a^b w(x)\,p_r(x)\,x^n\,\mathrm{d}x-\sum_{m=0}^{n-1}\gamma_{nm}\int_a^b w(x)\,p_r(x)\,p_m(x)\,\mathrm{d}x\,.\end{aligned} \tag{2.22}$$

This can also be written in the terms of weighted inner products as

$$\langle p_r,p_n\rangle=\langle p_r,x^n\rangle-\sum_{m=0}^{n-1}\gamma_{nm}\langle p_r,p_m\rangle\,. \tag{2.23}$$

Due to presumed orthogonality condition (2.9), from (2.23) and for $r=n$ it can be obtained

$$\langle p_n,p_n\rangle=\langle p_n,x^n\rangle\quad\text{or}\quad\langle p_r,p_r\rangle=\langle p_r,x^r\rangle\,. \tag{2.24}$$

In addition, from (2.23) and for $r<n$ it follows

$$\gamma_{nr}=\frac{\langle p_r,x^n\rangle}{\langle p_r,p_r\rangle}=\frac{\langle p_r,x^n\rangle}{\langle p_r,x^r\rangle},\quad r=0,...,n-1\,. \tag{2.25a}$$

It is convenient to replace index *r* with index *m* so that

$$\gamma_{nm} = \frac{\langle p_m, x^n \rangle}{\langle p_m, p_m \rangle} = \frac{\langle p_m, x^n \rangle}{\langle p_m, x^m \rangle}, \quad m = 0, ..., n-1 . \tag{2.25b}$$

Recursion starts with

$$\begin{aligned}
&p_0(x) = 1 \Rightarrow a_{0,0} = 1, \\
&\gamma_{1,0} = \frac{\langle p_0, x \rangle}{\langle p_0, 1 \rangle} = \frac{\langle a_{0,0}, x \rangle}{\langle a_{0,0}, 1 \rangle}, \\
&p_1(x) = x - \gamma_{1,0} p_0(x) \Rightarrow a_{1,1} = 1,\ a_{1,0} = -\gamma_{1,0} a_{0,0}, \\
&\gamma_{2,0} = \frac{\langle p_0, x^2 \rangle}{\langle p_0, 1 \rangle} = \frac{\langle a_{0,0}, x^2 \rangle}{\langle a_{0,0}, 1 \rangle}, \\
&\gamma_{2,1} = \frac{\langle p_1, x^2 \rangle}{\langle p_1, 1 \rangle} = \frac{\langle a_{1,1}x + a_{1,0}, x^2 \rangle}{\langle a_{1,1}x + a_{1,0}, 1 \rangle}, \\
&p_2(x) = x - \sum_{m=0}^{1} \gamma_{2,m} p_m(x) \Rightarrow a_{2,2} = 1,\ a_{2,1} = \dots .
\end{aligned} \tag{2.26}$$

For the calculation of inner products $\langle p_m, x^n \rangle$ and $\langle p_m, x^m \rangle$ it is necessary to determine coefficients a_{nr} of the orthogonal polynomials $p_n(x)$ (2.8). Substitution of the orthogonal polynomial $p_n(x)$ (2.8) into formula (2.21) gives

$$\sum_{r=0}^{n} a_{nr} x^r = x^n - \sum_{m=0}^{n-1} \gamma_{nm} \sum_{r=0}^{m} a_{mr} x^r . \tag{2.27}$$

Since,

$$\sum_{m=0}^{n-1} \gamma_{nm} \sum_{r=0}^{m} a_{mr} x^r = \sum_{r=0}^{n-1} \left(\sum_{m=r}^{n-1} \gamma_{nm} a_{mr} \right) x^r \tag{2.28}$$

the equation (2.27) can be transformed into

$$(a_{nn} - 1) x^n + \sum_{r=0}^{n-1} \left(a_{nr} + \sum_{m=r}^{n-1} \gamma_{nm} a_{mr} \right) x^r = 0 . \tag{2.29}$$

This equation is valid for any *x* only if the coefficients a_{nr} of polynomials $p_n(x)$ $(\forall n \geq 1)$, which are supposed to be orthogonal, are

$$\begin{aligned}
&a_{nn} = 1, \\
&a_{nr} = -\sum_{m=r}^{n-1} \gamma_{nm} a_{mr}, \quad r = 0, 1, ..., n-1.
\end{aligned} \tag{2.30}$$

It is now possible to calculate inner products $\langle p_m, x^n \rangle$ and $\langle f, p_n \rangle$. Note that the inner product $\langle p_m, x^m \rangle$ is a special case of $\langle p_m, x^n \rangle$. By substituting $p_n(x)$ (2.8) into inner products it can be obtained

$$\begin{aligned}\langle p_m, x^n \rangle &= \sum_{r=0}^{m} a_{mr} \langle x^r, x^n \rangle = \sum_{r=0}^{m} a_{mr} \int_a^b w(x)\, x^{r+n} \mathrm{d}x,\\ \langle f, p_n \rangle &= \sum_{r=0}^{n} a_{nr} \langle f, x^r \rangle = \sum_{r=0}^{n} a_{nr} \int_a^b w(x)\, f(x)\, x^r \mathrm{d}x.\end{aligned} \tag{2.31}$$

To apply developed formulas, it is convenient to introduce auxiliary variables

$$\begin{aligned}I_r &= \int_a^b w(x)\, x^r \mathrm{d}x,\\ J_r &= \int_a^b w(x)\, f(x)\, x^r \mathrm{d}x,\\ d_n &= \langle p_n, p_n \rangle = \langle p_n, x^n \rangle = \sum_{r=0}^{n} a_{nr} I_{r+n}.\end{aligned} \tag{2.32}$$

Therefore,

$$\begin{aligned}\gamma_{nm} &= \frac{\langle p_m, x^n \rangle}{\langle p_m, p_m \rangle} = \frac{1}{d_m} \sum_{r=0}^{m} a_{mr} I_{r+n}, \quad m = 0, \ldots, n-1,\\ \beta_n &= \frac{\langle f, p_n \rangle}{\langle p_n, p_n \rangle} = \frac{1}{d_n} \sum_{r=0}^{n} a_{nr} J_r.\end{aligned} \tag{2.33}$$

Complete procedure for determining coefficients a_{nr} of orthogonal polynomials $p_n(x)$, coefficients β_n and coefficients α_r (2.19) is given in Algorithm 2.1. Obtained coefficients α_r define resultant approximation polynomial in the form $\tilde{f}(x, \alpha) = \sum_{r=0}^{N-1} \alpha_r x^r$ (2.1) that is the most suitable form for further numerical manipulation.

Algorithm 2.1. Coefficients α_r for the orthogonal polynomial approximation with an arbitrary weighting function $w(x)$ on a continuous interval $[a,b]$

List of input variables: $N, a, b, *w, *f$ // "*"denotes pointers to $w(x)$ and $f(x)$
List of output variables: α_r // "//" denotes the beginning of a comment
// Polynomial $p_0(x)=1$
 $a_{0,0}=1$
 Calculate_and_store_integrals I_0, J_0 // Equation (2.32)
 $d_0 = I_0$
 $\beta_0 = J_0 / d_0$
// Polynomials $p_1(x)$, …, $p_{N-1}(x)$
 for $n = 1, ..., N-1$
  Calculate_and_store_integrals I_{2n-1}, I_{2n}, J_n // Equation (2.32)
  // Expansion of x^n into series of polynomials p_0, …, p_n (2.20), (2.33)
   for $m = 0, ..., n-1$
    $\gamma_{nm} = \frac{1}{d_m} \sum_{r=0}^{m} a_{mr} I_{r+n}$
   endfor
  // Coefficients a_{nr} (2.30) of orthogonal polynomial $p_n(x)$ (2.8)
   for $r = 0, ..., n-1$
    $a_{nr} = -\sum_{m=r}^{n-1} \gamma_{nm} a_{mr}$
   endfor
   $a_{nn} = 1$
  $d_n = \sum_{r=0}^{n} a_{nr} I_{r+n}$ // $d_n = \langle p_n, x^n \rangle$ (2.32)
  $\beta_n = \sum_{r=0}^{n} a_{nr} J_r / d_n$ // Generalised Fourier coefficients (2.33)
 endfor
// Calculating coefficients α_r of approximation polynomial $\tilde{f}(x,\alpha)$ (2.1)
 for $r = 0, ..., N-1$
  $\alpha_r = \sum_{n=r}^{N-1} \beta_n a_{nr}$ // Expression (2.19)
 endfor
end

2.2.2 Generating orthogonal polynomials by recursion

Another, more usual method for generating orthogonal polynomials $p_n(x)$ is the one using recurrence

$$p_0(x) = 1\,,$$

$$p_{-1}(x) = 0\,, \tag{2.34}$$

$$p_n(x) = (x - b_n)\,p_{n-1}(x) - c_{n-1}p_{n-2}(x)\,, \quad n \ge 1\,,$$

where b_n and c_n $(n = 1, 2, \ldots)$ are constants that have to be determined. So defined polynomials are standardised by the condition $p_n = x^n + \ldots$ (leading coefficient has value 1).

Recursion formula (2.34) can be multiplied by $w(x)\,p_m(x)$ and integrated over an interval $[a,b]$ to obtain

$$\begin{aligned}\int_a^b w(x)\,p_m(x)\,p_n(x)\,\mathrm{d}x &= \int_a^b w(x)\,x p_m(x)\,p_{n-1}(x)\,\mathrm{d}x - \\ &- b_n\int_a^b w(x)\,p_m(x)\,p_{n-1}(x)\,\mathrm{d}x - c_{n-1}\int_a^b w(x)\,p_m(x)\,p_{n-2}(x)\,\mathrm{d}x.\end{aligned} \tag{2.35}$$

This recursion formula can be expressed in the terms of the weighted inner products

$$\langle p_m, p_n\rangle = \langle x p_m, p_{n-1}\rangle - b_n\langle p_m, p_{n-1}\rangle - c_{n-1}\langle p_m, p_{n-2}\rangle\,, \quad n \ge 1\,. \tag{2.36}$$

In the first step, such polynomial $p_1(x)$ that is orthogonal to $p_0(x) = 1$ will be found from the condition that $\langle p_0, p_1\rangle = 0$. For $n = 1$ and $m = 0$, the recursion formula (2.36) gives

$$\underbrace{\langle p_0, p_1\rangle}_{0} = \langle x p_0, p_0\rangle - b_1\langle p_0, p_0\rangle - c_0\underbrace{\langle p_0, p_{-1}\rangle}_{0}\,, \tag{2.37}$$

where $\langle p_0, p_{-1}\rangle = \langle p_0, 0\rangle = 0$. Since constant c_0 is multiplied by zero, it can take any finite value. The most convenient one is $c_0 = 0$. In addition, due to prescribed orthogonality, the $\langle p_0, p_1\rangle = 0$.

Therefore,

$$b_1 = \frac{\langle x,1\rangle}{\langle 1,1\rangle} = \frac{\langle xp_0, p_0\rangle}{\langle p_0, p_0\rangle}, \qquad c_0 = 0. \tag{2.38}$$

In the second step, such polynomial $p_2(x)$ that is orthogonal to $p_1(x)$ and $p_0(x)$ will be found from the conditions that $\langle p_0, p_2\rangle = 0$ and $\langle p_1, p_2\rangle = 0$. For $n = 2$ and $m = 0,1$, the recursion (2.36) gives two equations

$$\underbrace{\langle p_0, p_2\rangle}_{0} = \langle xp_0, p_1\rangle - b_2\langle p_0, p_1\rangle - c_1\langle p_0, p_0\rangle,$$
$$\underbrace{\langle p_1, p_2\rangle}_{0} = \langle xp_1, p_1\rangle - b_2\langle p_1, p_1\rangle - c_1\langle p_1, p_0\rangle. \tag{2.39}$$

In addition, the polynomial p_1 defined by the coefficients b_1 and c_0 (2.38) is orthogonal to the polynomial p_0 and satisfies the condition $\langle p_0, p_1\rangle = \langle p_1, p_0\rangle = 0$; thus, from the equations (2.39) follow

$$b_2 = \frac{\langle xp_1, p_1\rangle}{\langle p_1, p_1\rangle}, \qquad c_1 = \frac{\langle xp_0, p_1\rangle}{\langle p_0, p_0\rangle}. \tag{2.40}$$

Suppose that polynomials $p_0(x)$ to $p_n(x)$ are orthogonal, so that they satisfy orthogonality conditions

$$\begin{aligned}&\langle p_0, p_{n-1}\rangle = 0, \quad \langle p_1, p_{n-1}\rangle = 0, \quad ..., \quad \langle p_{n-2}, p_{n-1}\rangle = 0,\\ &\langle p_0, p_n\rangle = 0, \quad \langle p_1, p_n\rangle = 0, \quad ..., \quad \langle p_{n-1}, p_n\rangle = 0,\end{aligned} \tag{2.41}$$

or shortly[1]

$$\begin{aligned}&\langle p_j, p_{n-1}\rangle = 0, \qquad j = 0,1,...,n-2,\\ &\langle p_j, p_n\rangle = 0, \qquad j = 0,1,...,n-1.\end{aligned} \tag{2.42}$$

[1] In general $\langle p_j, p_k\rangle = 0$ for $j < k \le n$.

It is now desired to find coefficients b_{n+1} and c_n that determine polynomial

$$p_{n+1}(x) = (x - b_{n+1}) p_n(x) - c_n p_{n-1}(x) , \tag{2.43}$$

which has to satisfy the orthogonality condition

$$\langle p_j, p_{n+1} \rangle = 0, \quad j = 0, 1, ..., n . \tag{2.44}$$

First of all, it will be verified that equation (2.44) is valid for $j = 0, .., n-2$, because of the orthogonality conditions (2.42). After that, such coefficients b_{n+1} and c_n will be found that satisfy equation (2.44) for $j = n-1$ and $j = n$.

From the recursion formula (2.36), from the orthogonality conditions (2.42) and for the $j = 0, .., n-2$, it follows

$$\langle p_j, p_{n+1} \rangle = \langle x p_j, p_n \rangle - b_{n+1} \underbrace{\langle p_j, p_n \rangle}_{0} - c_n \underbrace{\langle p_j, p_{n-1} \rangle}_{0} . \tag{2.45}$$

Term $x p_j$ is a polynomial of degree $j+1$ no greater than $n-1$, thus it can be expressed as a linear combination of the polynomials $p_r(x)$ $(r = 0, ..., n-1)$

$$x p_j(x) = \sum_{r=0}^{j+1} \gamma'_r p_r(x) . \tag{2.46}$$

Therefore, according to (2.45), for $j = 0, ..., n-2$, it follows

$$\langle p_j, p_{n+1} \rangle = \langle x p_j, p_n \rangle = \sum_{r=0}^{j+1} \gamma'_r \underbrace{\langle p_r, p_n \rangle}_{0} = 0 . \tag{2.47}$$

Hence, orthogonality condition $\langle p_j, p_{n+1} \rangle = 0$ (2.44) is satisfied for $j = 0, ..., n-2$, as it was expected.

Two remainder orthogonality conditions (2.44), those for $j = n$ and $j = n-1$:

$$\begin{aligned} \underbrace{\langle p_n, p_{n+1} \rangle}_{0} &= \langle x p_n, p_n \rangle - b_{n+1} \langle p_n, p_n \rangle - c_n \underbrace{\langle p_n, p_{n-1} \rangle}_{0} = 0, \\ \underbrace{\langle p_{n-1}, p_{n+1} \rangle}_{0} &= \langle x p_{n-1}, p_n \rangle - b_{n+1} \underbrace{\langle p_{n-1}, p_n \rangle}_{0} - c_n \langle p_{n-1}, p_{n-1} \rangle = 0 , \end{aligned} \tag{2.48}$$

are satisfied by

$$b_{n+1} = \frac{\langle xp_n, p_n \rangle}{\langle p_n, p_n \rangle},$$
$$c_n = \frac{\langle xp_{n-1}, p_n \rangle}{\langle p_{n-1}, p_{n-1} \rangle}. \tag{2.49}$$

Formula (2.49) for determining the coefficients c_n can be improved. From $\langle xp_{n-1}, p_n \rangle = \langle xp_n, p_{n-1} \rangle$ and from recursion formula (2.36) (and $m = n$), written in the form

$$\langle xp_n, p_{n-1} \rangle = \langle p_n, p_n \rangle + b_n \underbrace{\langle p_n, p_{n-1} \rangle}_{0} + c_{n-1} \underbrace{\langle p_n, p_{n-2} \rangle}_{0}, \tag{2.50}$$

follows the improved expression for calculating coefficients

$$c_n = \frac{\langle p_n, p_n \rangle}{\langle p_{n-1}, p_{n-1} \rangle}. \tag{2.51}$$

This improvement consists in using the inner product $\langle p_{n-1}, p_{n-1} \rangle$ already determined when previous coefficient $c_{n-1} = \langle p_{n-1}, p_{n-1} \rangle / \langle p_{n-2}, p_{n-2} \rangle$ has been calculated.

For the calculation of inner products it is necessary to determine coefficients a_{nr} of the orthogonal polynomials $p_n(x)$ (2.8). The coefficients a_{nr} of orthogonal polynomials $p_0(x) = 1$ and $p_1(x) = x - b_1$ are

$$a_{0,0} = 1,$$
$$a_{1,0} = -b_n,\ a_{1,1} = 1. \tag{2.52}$$

By substitution of orthogonal polynomial $p_n(x)$ (2.8) into recursion formula (2.34) it can be obtained

$$(\forall n \ge 2) \quad \sum_{r=0}^{n} a_{nr} x^r = (x - b_n) \sum_{r=0}^{n-1} a_{n-1,r} x^r - c_{n-1} \sum_{r=0}^{n-2} a_{n-2,r} x^r . \tag{2.53}$$

Since

$$x \sum_{r=0}^{n-1} a_{n-1,r} x^r = \sum_{r=0}^{n-1} a_{n-1,r} x^{r+1} = \sum_{r=1}^{n} a_{n-1,r-1} x^r , \tag{2.54}$$

it follows

$$(\forall n \geq 2) \quad \sum_{r=0}^{n} a_{nr} x^r = \sum_{r=1}^{n} a_{n-1,r-1} x^r - b_n \sum_{r=0}^{n-1} a_{n-1,r} x^r - c_{n-1} \sum_{r=0}^{n-2} a_{n-2,r} x^r . \quad (2.55)$$

By separation of coefficients, the coefficients a_{nr} $(\forall n \geq 2)$ can be calculated by recursion

$$\begin{aligned} & a_{n,0} = -b_n a_{n-1,0} - c_{n-1} a_{n-2,0}, \\ & (r = 1, ..., n-2) \quad a_{nr} = a_{n-1,r-1} - b_n a_{n-1,r} - c_{n-1} a_{n-2,r}, \\ & a_{n,n-1} = a_{n-1,n-2} - b_n a_{n-1,n-1} \\ & a_{nn} = a_{n-1,n-1}. \end{aligned} \quad (2.56)$$

It is now possible to calculate inner products $\langle f, p_n \rangle$, $\langle p_n, p_n \rangle$ and $\langle xp_n, p_n \rangle$. Inner products $\langle f, p_n \rangle$ and $\langle p_n, p_n \rangle$ are already defined by (2.31) and (2.32). By substituting $p_n(x)$ (2.8) into inner product $\langle xp_n, p_n \rangle$ it can be obtained

$$\langle xp_n, p_n \rangle = \sum_{r=0}^{n} \sum_{s=0}^{n} a_{nr} a_{ns} \int_a^b w(x)\, x^{r+s+1} \mathrm{d}x. \quad (2.57)$$

To apply developed formulas, it is convenient to introduce variables I_k, J_r, d_n and β_n already defined by (2.32) and (2.33). Therefore, according to (2.49) and (2.51) the coefficients

$$\begin{aligned} & b_n = \frac{\langle xp_{n-1}, p_{n-1} \rangle}{\langle p_{n-1}, p_{n-1} \rangle} = \frac{1}{d_{n-1}} \sum_{r=0}^{n-1} \sum_{s=0}^{n-1} a_{n-1,r} a_{n-1,s} I_{r+s+1}, \\ & c_{n-1} = \frac{\langle p_{n-1}, p_{n-1} \rangle}{\langle p_{n-2}, p_{n-2} \rangle} = \frac{d_{n-1}}{d_{n-2}}, \end{aligned} \quad (2.58)$$

can be calculated.

Complete procedure for determining coefficients a_{nr} of orthogonal polynomials, coefficients β_n and coefficients α_r (2.19) is given in Algorithm 2.2. Obtained coefficients α_r define resultant approximation polynomial $\tilde{f}(x, \alpha)$ (2.1) in the form that is the most suitable form for further numerical manipulation.

Algorithm 2.2. Coefficients α_r for the orthogonal polynomial approximation on a continuous interval $[a,b]$ by using recursion formula (2.34)

List of input variables: $N,a,b,*w,*f$ // "*"denotes pointers to $w(x)$ and $f(x)$
List of output variables: α_r // "//" denotes the beginning of a comment
// Polynomial $p_0(x)=1$
  $a_{0,0}=1$
  Calculate_and_store_integrals I_0, J_0 // Equation (2.32)
  $d_0 = I_0$; $\beta_0 = J_0/d_0$ // Equation (2.33)
// Polynomial $p_1(x) = x - b_1$
  Calculate_and_store_integrals I_1, I_2, J_1 // Equation (2.32)
  $b_1 = I_1/d_0$
  $a_{1,1}=1$; $a_{1,0}=-b_1$
  $d_1 = a_{1,0}I_1 + I_2$; $\beta_1 = (a_{1,0}J_0 + J_1)/d_1$ // Equation (2.33)
// Polynomials $p_2(x)$, …, $p_{N-1}(x)$
  for $n = 2, ..., N-1$
    Calculate_and_store_integrals I_{2n-1}, I_{2n}, J_n // Equation (2.32)
    $b_n = \sum_{r=0}^{n-1}\sum_{s=0}^{n-1} a_{n-1,r}a_{n-1,s}I_{r+s+1}/d_{n-1}$; $c_{n-1} = d_{n-1}/d_{n-2}$ // Equation (2.58)
    // Coefficients a_{nr} (2.56) of $p_n(x)$ (2.8)
      $a_{n,0} = -b_n a_{n-1,0} - c_{n-1}a_{n-2,0}$
      for $r = 1, ..., n-2$
        $a_{nr} = a_{n-1,r-1} - b_n a_{n-1,r} - c_{n-1}a_{n-2,r}$
      endfor
      $a_{n,n-1} = a_{n-1,n-2} - b_n a_{n-1,n-1}$; $a_{nn} = a_{n-1,n-1}$
    $d_n = \sum_{r=0}^{n} a_{nr}I_{r+n}$; $\beta_n = \sum_{r=0}^{n} a_{nr}J_r/d_n$ // Generalised Fourier coeff. (2.33)
  endfor
// Calculating coefficients α_r of approximation polynomial $\tilde{f}(x,\alpha)$ (2.1)
  for $r = 0, ..., N-1$
    $\alpha_r = \sum_{n=r}^{N-1} \beta_n a_{nr}$ // Equation (2.19)
  endfor
end

2.2.3 Legendre polynomials

Polynomials $P_n(x)$ ($n=0,1,2,\ldots$) that are orthogonal with respect to the *unit* weighting function $w(x)=1$ on the interval $[-1,1]$ and standardised with the condition $P_n(1)=1$, are called *Legendre polynomials*[2].

They are given by Rodrigue's formula

$$\begin{aligned} &P_0(x)=1, \\ &(\forall n\geq 1)\quad P_n(x)=\frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n, \end{aligned} \tag{2.59}$$

and by explicit expression[3] [8]:

$$P_n(x)=\frac{1}{2^n}\sum_{m=0}^{\mathrm{int}(n/2)}(-1)^m\binom{n}{m}\binom{2n-2m}{n}x^{n-2m} \tag{2.60}$$

that yields to

$$\begin{aligned} P_n(x)=\frac{(2n-1)(2n-3)\ldots 1}{n!}\Bigg[x^n-\frac{n(n-1)}{2(2n-1)}x^{n-2}+ \\ +\frac{n(n-1)(n-2)(n-3)}{2\cdot 4(2n-1)(2n-3)}x^{n-4}-\ldots\Bigg]. \end{aligned} \tag{2.61}$$

The general recursion relation is

$$(\forall n\geq 1)\quad P_n(x)=\frac{2n-1}{n}xP_{n-1}(x)-\frac{n-1}{n}P_{n-2}(x), \tag{2.62}$$

starting with $P_0(x)=1$.

---

[2] The general solution of *Legendre's differential equation* $(1-x^2)y''-2xy'+n(n+1)y=0$ for $n=0,1,2,3,\ldots$ is linear combination $y=c_1P_n+c_2Q_n$ of *Legendre polynomials* P_n and *Legendre functions of the second kind* $Q_n=\frac{1}{2}P_n\ln\frac{1+x}{1-x}-\sum_{k=1}^{n}\frac{1}{k}P_{k-1}P_{n-k}$ for $|x|<1$.

[3] $\mathrm{int}(n/2)$ means integer part of $n/2$.

Example 2.1. First few Legendre polynomials are

$$\begin{aligned} &P_0 = 1, && P_4 = \frac{1}{8}(35x^4 - 30x^2 + 3), \\ &P_1 = x, && P_5 = \frac{1}{8}(63x^5 - 70x^3 + 15x), \\ &P_2 = \frac{1}{2}(3x^2 - 1), && P_6 = \frac{1}{16}(231x^6 - 693x^4 + 105x^2 - 5), \\ &P_3 = \frac{1}{2}(5x^3 - 3x), && P_7 = \frac{1}{16}(429x^7 - 693x^5 + 315x^3 - 35x). \end{aligned} \tag{2.63}$$

Plots of few Legendre polynomials are presented on Fig. 2.1.

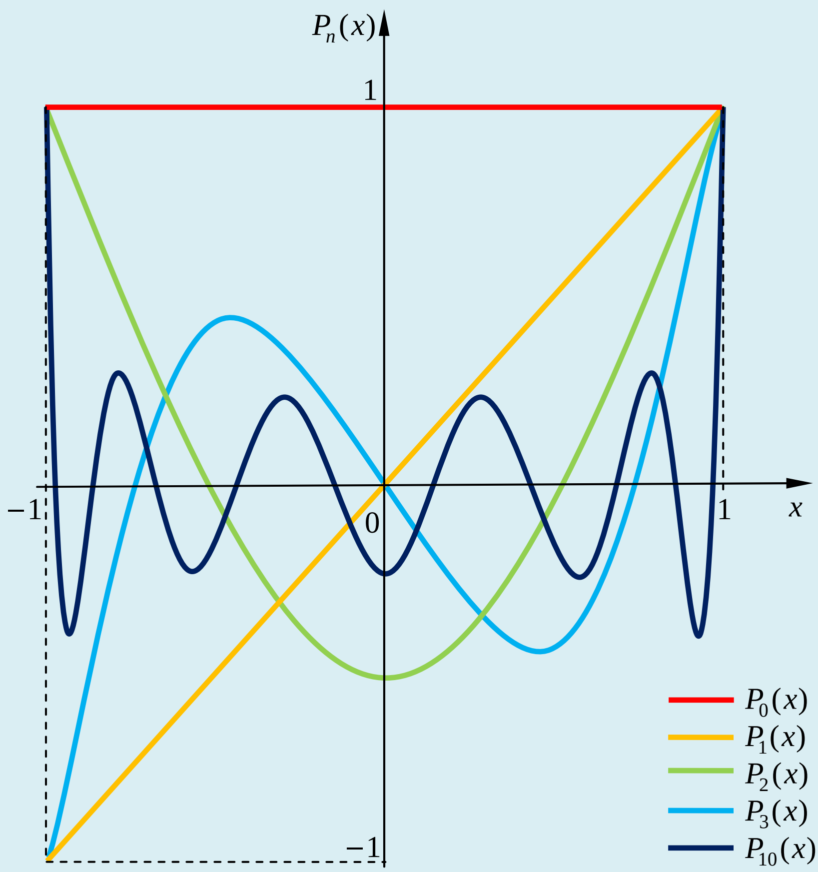

Fig. 2.1. *Plot of few Legendre polynomials*

Due to their orthogonality, the Legendre polynomials satisfy the expression

$$\langle P_n, P_m \rangle = \int_{-1}^{1} P_n(x) P_m(x)\,\mathrm{d}x = \begin{cases} 0, & m \neq n, \\ 2/(2n+1), & m = n. \end{cases} \tag{2.64}$$

Other properties of Legendre polynomials:

1. All roots are real and placed on the interval $[-1,1]$,
2. $P_n(1) = 1$ and $P_n(-1) = (-1)^n$,
3. $P_n(-x) = (-1)^n P_n(x)$.
4. Monomials x^n are orthogonal to the Legendre polynomials, i.e.

$$\int_{-1}^{1} x^n P_m(x)\mathrm{d}x = \begin{cases} 0, & m \neq n, \\ \dfrac{2^{n+1}(n!)^2}{(2n+1)!}, & m = n. \end{cases} \tag{2.65}$$

2.2.4 Associated Legendre polynomials

Polynomials defined in terms of the Legendre polynomials $P_n(x)$ by

$$P_n^k(x) = (1-x^2)^{k/2} \frac{d^k}{dx^k} P_n(x), \quad k = 1, 2, \ldots, \tag{2.66}$$

are called *associated Legendre polynomials*[4]. The general recursion relation is

$$(\forall n \geq 2) \quad P_n^k(x) = \frac{2n-1}{n} x P_{n-1}^k(x) - \frac{n-1}{n} P_{n-2}^k(x). \tag{2.67}$$

Note that order of the polynomial $P_n^k(x)$ is $n-k$. If $n<k$ the polynomial $P_n^k(x)$ does *not* have negative order, it is equal to zero (i.e. $P_n^k(x) = 0$, $n<k$).

---

[4] The general solution of *Legendre's associated differential equation* $(1-x^2)y'' - 2xy' + [n(n+1) - k^2/(1-x^2)]y = 0$ (obtained from Laplace's differential equation expressed in spherical coordinates), where n and k are nonnegative integers, is linear combination $y = c_1 P_n^k(x) + c_2 Q_n^k(x)$ of *associated Legendre polynomials* P_n^k and *associated Legendre functions of the second kind* $Q_n^k = (1-x^2)^{k/2} d^k Q_n / dx^k$.

Like Legendre polynomials, set of polynomials $P_n^k(x)$ for the particular k are also orthogonal with respect to the unit weighting function $w(x)=1$ on the interval $[-1,1]$, i.e.

$$\langle P_m^k, P_n^k \rangle = \int_{-1}^{1} P_m^k(x) P_n^k(x)\,\mathrm{d}x = 0, \quad m \neq n,$$
$$\langle P_n^k, P_n^k \rangle = \int_{-1}^{1} [P_n^k(x)]^2\,\mathrm{d}x = \begin{cases} \dfrac{2}{2n+1}\dfrac{(n+k)!}{(n-k)!}, & n \geq k, \\ 0, & n < k. \end{cases} \tag{2.68}$$

2.2.5 Approximation with Legendre polynomials

Let function $f(x)$ be approximated on the interval $[-1,1]$ with approximation function

$$\tilde{f}(x,\beta) = \sum_{n=0}^{N-1} \beta_n P_n(x), \quad -1 \leq x \leq 1, \tag{2.69}$$

by using Legendre polynomials $P_n(x)$. Generalised Fourier coefficients β_n can be obtained by substituting $p_n(x) = P_n(x)$ into expression (2.10) as

$$\beta_n = \frac{\langle f, P_n \rangle}{\langle P_n, P_n \rangle} = \frac{2}{2n+1} \int_{-1}^{1} f(x)\, P_n(x)\,\mathrm{d}x\,. \tag{2.70}$$

By substituting Legendre polynomials

$$P_n(x) = \sum_{r=0}^{n} a_{nr} x^r = a_{n,n} x^n + a_{n,n-1} x^{n-1} + \ldots + a_{n,1} x + a_{n,0}\,, \tag{2.71}$$

into the inner product $\langle f, P_n \rangle$ it can be obtained

$$\beta_n = \frac{2}{2n+1} \sum_{r=0}^{n} a_{nr} \langle f, x^r \rangle = \frac{2}{2n+1} \sum_{r=0}^{n} a_{nr} \int_{-1}^{1} f(x)\, x^r\,\mathrm{d}x\,. \tag{2.72}$$

By substituting polynomials $P_n(x)$ (2.71) into approximation function $\tilde{f}(x,\beta)$ it can be expressed in the form of polynomial $\tilde{f}(x,\alpha)$ (2.1) of degree $N-1$ which is determined with coefficients α_r (2.19).

Coefficients a_{nr} can be obtained by substituting polynomial $P_n(x)$ (2.71) into recursion formula (2.62):

$$(\forall n \geq 2) \quad \sum_{r=0}^{n} a_{nr} x^r = \frac{2n-1}{n} x \sum_{r=0}^{n-1} a_{n-1,r} x^r - \frac{n-1}{n} \sum_{r=0}^{n-2} a_{n-2,r} x^r \,. \tag{2.73}$$

By rearranging summation

$$x \sum_{r=0}^{n-1} a_{n-1,r} x^r = \sum_{r=0}^{n-1} a_{n-1,r} x^{r+1} = \sum_{r=1}^{n} a_{n-1,r-1} x^r \tag{2.74}$$

it can be obtained

$$(\forall n \geq 2) \quad \sum_{r=0}^{n} a_{nr} x^r = \frac{2n-1}{n} \sum_{r=1}^{n} a_{n-1,r-1} x^r - \frac{n-1}{n} \sum_{r=0}^{n-2} a_{n-2,r} x^r \,. \tag{2.75}$$

Coefficients a_{nr} are independent of *x*; thus, from (2.75) follow

$$\begin{aligned} & a_{n,0} = -\frac{n-1}{n} a_{n-2,0} \,, \\ & (r = 1, \ldots, n-2) \quad a_{nr} = \frac{2n-1}{n} a_{n-1,r-1} - \frac{n-1}{n} a_{n-2,r} \,, \\ & a_{n,n-1} = \frac{2n-1}{n} a_{n-1,n-2} \,, \\ & a_{nn} = \frac{2n-1}{n} a_{n-1,n-1} . \end{aligned} \tag{2.76}$$

To apply developed formulas, it is convenient to introduce variable

$$J_r = \langle f, x^r \rangle = \int_{-1}^{1} f(x)\, x^r \, \mathrm{d}x \,. \tag{2.77}$$

Therefore,

$$\beta_n = \frac{2}{2n+1} \sum_{r=0}^{n} a_{nr} J_r \,. \tag{2.78}$$

Procedure for calculating coefficients a_{nr} of Legendre polynomials $P_n(x)$, generalised Fourier coefficients β_n and coefficients α_r (2.19) of resultant approximation polynomial $\tilde{f}(x, \alpha)$ (2.1) is given in Algorithm 2.3.

Algorithm 2.3. Coefficients α_r in the Legendre polynomial approximation

List of input variables: N, *f // "*" denotes pointer to $f(x)$
List of output variables: α_r // "//" denotes the beginning of a comment

// Polynomial $P_0(x)=1$
$a_{0,0}=1$
$J_0=\int_{-1}^{1} f(x)\,\mathrm{d}x$ // Equation (2.77)
$\beta_0=2J_0$ // Equation (2.78)
// Polynomial $P_1(x)=x$
$a_{1,1}=1$; $a_{1,0}=0$
$J_1=\int_{-1}^{1} f(x)\,x\,\mathrm{d}x$ // Equation (2.77)
$\beta_1=2J_1/3$ // Equation (2.78)
// Polynomials $P_2(x)$, …, $P_{N-1}(x)$
for $n=2,\ldots,N-1$
// Calculate coefficients a_{nr} (2.76) of $P_n(x)$ (2.71)
$a_{n,0}=-(n-1)a_{n-2,0}/n$
for $r=1,\ldots,n-2$
$a_{nr}=((2n-1)a_{n-1,r-1}-(n-1)a_{n-2,r})/n$
endfor
$a_{n,n-1}=(2n-1)a_{n-1,n-2}/n$; $a_{nn}=(2n-1)a_{n-1,n-1}/n$
$J_n=\int_{-1}^{1} f(x)\,x^n\,\mathrm{d}x$ // Equation (2.77)
$\beta_n=\frac{2}{2n+1}\sum_{r=0}^{n} a_{nr}J_r$ // Generalised Fourier coefficient (2.78)
endfor
// Calculating coefficients α_r of approximation polynomial $\tilde{f}(x,\alpha)$ (2.1)
for $r=0,\ldots,N-1$
$\alpha_r=\sum_{n=r}^{N-1}\beta_n a_{nr}$ // Equation (2.19)
endfor
end

2.2.6 Shifted Legendre polynomials

It is often convenient to use the interval $[0,1]$ instead of the interval $[-1,1]$. The polynomials $P_n^*(x)$ $(n = 0,1,2,\ldots)$ that are orthogonal with respect to the *unit* weighting function $w(x) = 1$ on the interval $[0,1]$ and standardised with condition $P_n^*(1) = 1$, are called *shifted Legendre polynomials.* All expressions related to the ordinary Legendre polynomials can be adapted by substitution

$$x \to 2x - 1. \tag{2.79}$$

The general recursion relation is

$$(\forall n \geq 1) \quad P_n^*(x) = \frac{2n-1}{n}(2x-1)P_{n-1}^*(x) - \frac{n-1}{n}P_{n-2}^*(x), \tag{2.80}$$

starting with $P_0^*(x) = 1$.

Example 2.2. First few shifted Legendre polynomials are [9]:

$$\begin{aligned}
P_0^* &= 1, \\
P_1^* &= 2x - 1, \\
P_2^* &= 6x^2 - 6x + 1, \\
P_3^* &= 20x^3 - 30x^2 + 12x - 1, \\
P_4^* &= 70x^4 - 140x^3 + 90x^2 - 20x + 1, \\
P_5^* &= 252x^5 - 630x^4 + 560x^3 - 210x^2 + 30x - 1, \\
P_6^* &= 924x^6 - 2772x^5 + 3150x^4 - 1680x^3 + 420x^2 - 42x + 1, \\
P_7^* &= 3432x^7 - 12012x^6 + 16632x^5 - 11550x^4 + \\
&\quad + 4200x^3 - 756x^2 + 56x - 1, \\
P_8^* &= 12870x^8 - 51480x^7 + 84084x^6 - 72072x^5 + \\
&\quad + 34650x^4 - 9240x^3 + 1260x^2 - 72x + 1, \\
P_9^* &= 48620x^9 - 218790x^8 + 411840x^7 - 420420x^6 + \\
&\quad + 252252x^5 - 90090x^4 + 18480x^3 - 1980x^2 + 90x - 1, \\
P_{10}^* &= 184756x^{10} - 923780x^9 + 1969110x^8 - 2333760x^7 + 1681680x^6 - \\
&\quad - 756756x^5 + 210210x^4 - 34320x^3 + 2970x^2 - 110x + 1.
\end{aligned} \tag{2.81}$$

Due to their orthogonality, shifted Legendre polynomials satisfy expression

$$\langle P_n^*, P_m^* \rangle = \int_0^1 P_n^*(x) P_m^*(x)\,\mathrm{d}x = \begin{cases} 0 & m \neq n, \\ 1/(2n+1) & m = n. \end{cases} \tag{2.82}$$

2.2.7 Approximation with shifted Legendre polynomials

Let a function $f(x)$ be approximated on the interval [0,1] with approximation function

$$\tilde{f}(x, \beta^*) = \sum_{n=0}^{N-1} \beta_n^* P_n^*(x), \quad 0 \leq x \leq 1, \tag{2.83}$$

by using shifted Legendre polynomials $P_n^*(x)$. Generalised Fourier coefficients β_n^* can be obtained by substituting $p_n(x) = P_n^*(x)$ into expression (2.10) as

$$\beta_n^* = \frac{\langle f, P_n^* \rangle}{\langle P_n^*, P_n^* \rangle} = \frac{1}{2n+1} \int_0^1 f(x)\, P_n^*(x)\,\mathrm{d}x\,. \tag{2.84}$$

By substituting shifted Legendre polynomials

$$P_n^*(x) = \sum_{r=0}^{n} a_{nr} x^r = a_{nn}^* x^n + a_{n,n-1}^* x^{n-1} + \ldots + a_{n,1}^* x + a_{n,0}^*\,, \tag{2.85}$$

into inner product $\langle f, P_n^* \rangle$ it can be obtained

$$\beta_n^* = \frac{1}{2n+1} \sum_{r=0}^{n} a_{nr}^* \langle f, x^r \rangle = \frac{2}{2n+1} \sum_{r=0}^{n} a_{nr}^* \int_0^1 f(x)\, x^r\,\mathrm{d}x\,. \tag{2.86}$$

By substituting polynomials $P_n^*(x)$ (2.85) into (2.83), the approximation function $\tilde{f}(x, \beta^*)$ can be expressed in the form of polynomial $\tilde{f}(x, \alpha)$ (2.1) of degree $N-1$ which is determined with coefficients α_r (2.19).

Coefficients a_{nr}^* can be obtained by substituting polynomial $P_n^*(x)$ (2.85) into recursion formula (2.80):

$$(\forall n \geq 2) \quad \sum_{r=0}^{n} a_{nr}^* x^r = \frac{2n-1}{n}(2x-1) \sum_{r=0}^{n-1} a_{n-1,r}^* x^r - \frac{n-1}{n} \sum_{r=0}^{n-2} a_{n-2,r}^* x^r\,. \tag{2.87}$$

By rearranging summation

$$x\sum_{r=0}^{n-1} a^*_{n-1,r} x^r = \sum_{r=0}^{n-1} a^*_{n-1,r} x^{r+1} = \sum_{r=1}^{n} a^*_{n-1,r-1} x^r \tag{2.88}$$

it can be obtained

$$\begin{aligned}(\forall n \ge 2)\quad \sum_{r=0}^{n} a^*_{nr} x^r &= 2\frac{2n-1}{n}\sum_{r=1}^{n} a^*_{n-1,r-1} x^r - \\ &\quad -\frac{2n-1}{n}\sum_{r=0}^{n-1} a^*_{n-1,r} x^r - \frac{n-1}{n}\sum_{r=0}^{n-2} a^*_{n-2,r} x^r .\end{aligned} \tag{2.89}$$

Coefficients a^*_{nr} are independent of *x*; thus, from (2.89) follows

$$\begin{aligned}&a^*_{n,0} = -\frac{2n-1}{n} a^*_{n-1,0} - \frac{n-1}{n} a^*_{n-2,0},\\ &(\forall r = 1,\dots,n-2)\quad a^*_{nr} = \frac{2n-1}{n}(2a^*_{n-1,r-1} - a^*_{n-1,r}) - \frac{n-1}{n} a^*_{n-2,r},\\ &a^*_{n,n-1} = \frac{2n-1}{n}(2a^*_{n-1,n-2} - a^*_{n-1,n-1}),\\ &a^*_{nn} = 2\frac{2n-1}{n} a^*_{n-1,n-1}.\end{aligned} \tag{2.90}$$

To apply developed formulas, it is convenient to introduce variable

$$J^*_r = \langle f, x^r \rangle = \int_0^1 f(x)\, x^r \, \mathrm{d}x . \tag{2.91}$$

Therefore,

$$\beta^*_n = \frac{1}{2n+1}\sum_{r=0}^{n} a^*_{nr} J^*_r . \tag{2.92}$$

The procedure for calculating coefficients a^*_{nr} of shifted Legendre polynomials $P^*_n(x)$, generalised Fourier coefficients β^*_n and coefficients α_r (2.19) of resultant approximation polynomial $\tilde{f}(x,\alpha)$ (2.1) is given in Algorithm 2.4.

Algorithm 2.4. Coefficients α_r in the approximation with shifted Legendre polynomials

List of input variables: N, $*f$ // "*" denotes pointer to $f(x)$

List of output variables: α_r // "//" denotes the beginning of a comment

// Polynomial $P_0^*(x) = 1$

$a_{0,0}^* = 1$

$J_0^* = \int_0^1 f(x)\,\mathrm{d}x$ // Equation (2.91)

$\beta_0^* = J_0^*$ // Equation (2.92)

// Polynomial $P_1^*(x) = 2x - 1$

$a_{1,1}^* = 2$; $a_{1,0}^* = -1$

$J_1^* = \int_0^1 f(x)\,x\,\mathrm{d}x$ // Equation (2.91)

$\beta_1^* = (2J_1^* - J_0^*)/3$ // Equation (2.92)

// Polynomials $P_2^*(x)$, …, $P_{N-1}^*(x)$

for $n = 2, ..., N-1$

// Calculate coefficients a_{nr}^* (2.90) of $P_n^*(x)$ (2.85)

$a_{n,0}^* = -(2n-1)a_{n-1,0}^*/n - (n-1)a_{n-2,0}^*/n$

for $r = 1, ..., n-2$

$a_{nr}^* = ((2n-1)(2a_{n-1,r-1}^* - a_{n-1,r}^*) - (n-1)a_{n-2,r}^*)/n$

endfor

$a_{n,n-1}^* = (2n-1)(2a_{n-1,n-2}^* - a_{n-1,n-1}^*)/n$; $a_{nn}^* = 2(2n-1)a_{n-1,n-1}^*/n$

$J_n^* = \int_0^1 f(x)\,x^n\,\mathrm{d}x$ // Equation (2.91)

$\beta_n^* = \dfrac{1}{2n+1}\sum_{r=0}^{n} a_{nr}^* J_r^*$ // Generalised Fourier coefficient (2.92)

endfor

// Calculating coefficients α_r of approximation polynomial $\tilde{f}(x,\alpha)$ (2.1)

for $r = 0, ..., N-1$

$\alpha_r = \sum_{n=r}^{N-1} \beta_n^* a_{nr}^*$ // Equation (2.19)

endfor

end

2.2.8 Other use of Legendre polynomials

Legendre polynomials can also be used in finding some other sets of orthogonal functions, e.g. by substitution

$$x = \cos\theta\,. \tag{2.93}$$

Since

$$\mathrm{d}x = \mathrm{d}\cos\theta = -\sin\theta\,\mathrm{d}\theta\,, \tag{2.94}$$

from (2.64) follows that functions $V_n(\theta) = P_n(\cos\theta)$ $(n = 0, 1, 2, \ldots)$ are orthogonal with respect to the weighting function $w(\theta) = \sin\theta$ on the interval $[-\pi, \pi]$, i.e. functions $V_n(\theta)$ satisfy condition of orthogonality

$$\langle V_n, V_m \rangle = \int_{-\pi}^{\pi} \sin\theta\, V_n(\theta) V_m(\theta) \mathrm{d}\theta = \begin{cases} 0, & m \neq n, \\ \dfrac{-2}{2n+1}, & m = n. \end{cases} \tag{2.95}$$

By substituting $x = \cos\theta$ (2.93) into (2.63) it can be obtained:

$$\begin{aligned}
V_0(\theta) &= 1, \\
V_1(\theta) &= \cos\theta, \\
V_2(\theta) &= \frac{1}{4}(3\cos 2\theta + 1), \\
V_3(\theta) &= \frac{1}{8}(5\cos 3\theta + 3\cos\theta), \\
V_4(\theta) &= \frac{1}{64}(35\cos 4\theta + 20\cos 2\theta + 9), \\
V_5(\theta) &= \frac{1}{128}(63\cos 5\theta + 35\cos 3\theta + 30\cos\theta), \\
V_6(\theta) &= \frac{1}{512}(231\cos 6\theta + 126\cos 4\theta + 105\cos 2\theta + 50).
\end{aligned} \tag{2.96}$$

The similar orthogonal sets of functions can be obtained by various substitutions. For example, substitution $x = \frac{1}{\pi}\arccos y$ leads to the Chebyshev polynomials $T_n(y) = \cos(n \arccos y)$ that are described in Chapter 4.

2.2.9 Jacobi polynomials

Polynomials $Q_n^{\alpha\beta}(x)$ ($n = 0, 1, 2, \ldots$; $\alpha > -1$; $\beta > -1$) that are orthogonal with respect to the weighting function

$$w^{\alpha\beta}(x) = (1-x)^{\alpha}(1+x)^{\beta} \tag{2.97}$$

on the interval $[-1,1]$, are called *Jacobi polynomials* [10, 11]. They are given by Rodrigue's formula

$$\begin{aligned} &Q_0^{\alpha\beta}(x) = 1, \\ &(\forall n \ge 1) \quad Q_n^{\alpha\beta}(x) = \frac{(-1)^n}{2^n n!(1-x)^{\alpha}(1+x)^{\beta}} \frac{\mathrm{d}^n}{\mathrm{d}x^n}(1-x)^{n+\alpha}(1+x)^{n+\beta}, \end{aligned} \tag{2.98}$$

and by explicit expression[5]

$$Q_n^{\alpha\beta}(x) = \frac{1}{2^n}\sum_{m=0}^{n}\binom{n+\alpha}{m}\binom{n+\beta}{n-m}(x-1)^{n-m}(1+x)^m. \tag{2.99}$$

The Jacobi polynomials satisfy recurrence relation

$$(\forall n \ge 2) \quad Q_n^{\alpha\beta}(x) = (A_n x + B_n)Q_{n-1}^{\alpha\beta}(x) - C_n Q_{n-2}^{\alpha\beta}(x), \tag{2.100}$$

where

$$\begin{aligned} A_n &= \frac{(2n+\alpha+\beta-1)(2n+\alpha+\beta)}{2n(n+\alpha+\beta)}, \\ B_n &= \frac{(\alpha+\beta)(\alpha-\beta)(2n+\alpha+\beta-1)}{2n(n+\alpha+\beta)(2n+\alpha+\beta-2)}, \\ C_n &= \frac{(n+\alpha-1)(n+\beta-1)(2n+\alpha+\beta)}{n(n+\alpha+\beta)(2n+\alpha+\beta-2)}. \end{aligned} \tag{2.101}$$

Example 2.3. First few Jacobi polynomials are

$$\begin{aligned} Q_0^{\alpha\beta} &= 1, \\ Q_1^{\alpha\beta} &= \frac{1}{2}[2(\alpha+1) + (\alpha+\beta+2)(x-1)], \\ Q_2^{\alpha\beta} &= \frac{1}{8}[4(\alpha+1)(\alpha+2) + 4(\alpha+\beta+3)(\alpha+2)(x-1) + \\ &\qquad + (\alpha+\beta+3)(\alpha+\beta+4)(x-1)^2]. \end{aligned} \tag{2.102}$$

---

[5] Jacobi polynomials are also solutions of differential equation $(1-x^2)y'' + (\beta - \alpha - {}$ ${}-(\alpha+\beta+2)x)y' + n(n+\alpha+\beta+1)y = 0$.

Due to their orthogonality, Jacobi polynomials satisfy expressions[6]

$$\langle Q_n^{\alpha\beta}, Q_m^{\alpha\beta}\rangle = \int_{-1}^{1} w^{\alpha\beta}(x) Q_n^{\alpha\beta}(x) Q_m^{\alpha\beta}(x)\,\mathrm{d}x = 0, \quad n \neq m,$$

$$\langle Q_n^{\alpha\beta}, Q_n^{\alpha\beta}\rangle = \int_{-1}^{1} w^{\alpha\beta}(x) [Q_n^{\alpha\beta}(x)]^2\,\mathrm{d}x = \tag{2.103}$$

$$= \frac{2^{\alpha+\beta+1}}{(2n+\alpha+\beta+1)} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+1)}.$$

The polynomials have symmetry relation

$$Q_n^{\alpha\beta}(-x) = (-1)^n Q_n^{\beta\alpha}(x)\,. \tag{2.104}$$

Values of polynomials at endpoints of the interval $[-1,1]$:

$$Q_n^{\alpha\beta}(-1) = (-1)^n \binom{n+\beta}{n} = \frac{\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(\beta+1)}\,, \tag{2.105}$$

$$Q_n^{\alpha\beta}(1) \quad = \quad \binom{n+\alpha}{n} = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}\,, \tag{2.106}$$

are independent of α or β respectively.

Jacobi series

$$f(x) = \sum_{n=0}^{\infty} \beta_n Q_n^{\alpha\beta}(x) \tag{2.107}$$

has coefficients

$$\beta_n = \frac{\langle f, Q_n^{\alpha\beta}\rangle}{\langle Q_n^{\alpha\beta}, Q_n^{\alpha\beta}\rangle}\,. \tag{2.108}$$

Herein

$$\langle f, Q_n^{\alpha\beta}\rangle = \int_{-1}^{1} w^{\alpha\beta}(x) f(x) Q_n^{\alpha\beta}(x)\mathrm{d}x = \tag{2.109}$$

$$= \frac{1}{2^n n!} \int_{-1}^{1} w^{\alpha\beta}(x) f^{(n)}(x)(1-x^2)^n\,\mathrm{d}x.$$

[6] $\Gamma(n)$ is the *gamma function* (see Appendix B.1).

In the special cases, when α and β take some characteristic values, the Jacobi polynomials become *ultraspherical polynomials* ($\alpha = \beta$), *Legendre polynomials* ($\alpha = \beta = 0$), *Chebyshev polynomials* ($\alpha = \beta = -1/2$) and *Chebyshev polynomials of the second kind* ($\alpha = \beta = 1/2$). According to usual symbols used in denoting these polynomials (see Table 2.1), there are

$$
\begin{aligned}
&C_n^{\alpha}(x) = Q_n^{\alpha\alpha}(x), && \text{ultraspherical (Gegenbauer)},\\
&P_n(x) = C_n^{0}(x) = Q_n^{0,0}(x), && \text{Legendre},\\
&T_n(x) = a'_n C_n^{-1/2}(x) = a'_n Q_n^{-1/2,-1/2}(x), && \text{Chebyshev},\\
&U_n(x) = a''_n C_n^{1/2}(x) = a''_n Q_n^{1/2,1/2}(x), && \text{Chebyshev 2}^{\text{nd}}\text{ kind}.
\end{aligned}
\tag{2.110}
$$

Constants a'_n and a''_n adjust polynomials $C_n^{-1/2}$ and $C_n^{1/2}$ to get Chebyshev polynomials T_n and U_n in standardised form.

Therefore, ultraspherical polynomials are a subclass of Jacobi polynomials, while Legendre and Chebyshev polynomials are subclasses of ultraspherical polynomials.

Example 2.4. First few ultraspherical, Legendre and Chebyshev polynomials:

$$
\begin{aligned}
C_0^{\alpha} &= Q_0^{\alpha\alpha} = 1,\\
C_1^{\alpha} &= Q_1^{\alpha\alpha} = (\alpha+1)x,\\
C_2^{\alpha} &= Q_2^{\alpha\alpha} = \frac{1}{4}(\alpha+2)[2(\alpha+1)+\\
&\qquad + 2(2\alpha+3)(x-1) + (2\alpha+3)(x-1)^2],
\end{aligned}
\tag{2.111}
$$

$$
\begin{aligned}
&P_0 = C_0^0 = 1, && P_1 = C_1^0 = x, && P_2 = C_2^0 = \frac{1}{2}(3x^2-1),\\
&T_0 = C_0^{-1/2} = 1, && T_1 = 2C_1^{-1/2} = x, && T_2 = \frac{8}{3}C_2^{-1/2} = 2x^2-1,\\
&U_0 = C_0^{1/2} = 1, && U_1 = \frac{4}{3}C_1^{1/2} = 2x, && U_2 = \frac{8}{5}C_2^{1/2} = 4x^2-1.
\end{aligned}
\tag{2.112}
$$

Procedure for calculation of generalised Fourier coefficients β_n can be developed by substituting Jacobi polynomials expressed in the form

$$Q_n^{\alpha\beta} = \sum_{r=0}^{n} a_{nr} x^r = a_{nn} x^n + a_{n,n-1} x^{n-1} + \ldots + a_{n,1} x + a_{n,0} \tag{2.113}$$

into the inner product $\langle f, Q_n^{\alpha\beta} \rangle$. The result is

$$\langle f, Q_n^{\alpha\beta} \rangle = \sum_{r=0}^{n} a_{nr} \langle f, x^r \rangle = \sum_{r=0}^{n} a_{nr} \int_{-1}^{1} w^{\alpha\beta}(x)\ f(x)\, x^r\ \mathrm{d}x\,. \tag{2.114}$$

To apply developed formulas, it is convenient to introduce variables

$$d_n = \langle Q_n^{\alpha\beta}, Q_n^{\alpha\beta} \rangle = \frac{2^{\alpha+\beta+1}}{(2n+\alpha+\beta+1)} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+1)}\,, \tag{2.115}$$

$$J_r = \langle f, x^r \rangle = \int_{-1}^{1} w^{\alpha\beta}(x)\ f(x)\, x^r\ \mathrm{d}x\,. \tag{2.116}$$

Therefore,

$$\beta_n = \frac{\langle f, Q_n^{\alpha\beta} \rangle}{\langle Q_n^{\alpha\beta}, Q_n^{\alpha\beta} \rangle} = \frac{1}{d_n} \sum_{r=0}^{n} a_{nr} J_r\,. \tag{2.117}$$

For the calculation of the generalised Fourier coefficients β_n, it is necessary to determine coefficients a_{nr} of the Jacobi polynomials $Q_n^{\alpha\beta}(x)$. The coefficients a_{nr} of the first two Jacobi polynomials $Q_0^{\alpha\beta}(x) = 1$ and $Q_1^{\alpha\beta}(x) = (\alpha+\beta+2)x/2 + {} + (\alpha-\beta)/2$ are

$$\begin{aligned} &a_{0,0} = 1, \\ &a_{1,0} = \frac{1}{2}(\alpha-\beta), \quad a_{1,1} = \frac{1}{2}(\alpha+\beta+2). \end{aligned} \tag{2.118}$$

Substitution of polynomials $Q_n^{\alpha\beta}$ (2.113) into recursion formula (2.100) gives

$$(\forall n \geq 2) \quad \sum_{r=0}^{n} a_{nr} x^r = (A_n x - B_n) \sum_{r=0}^{n-1} a_{n-1,r} x^r - C_n \sum_{r=0}^{n-2} a_{n-2,r} x^r\,. \tag{2.119}$$

By rearranging summation

$$x\sum_{r=0}^{n-1} a_{n-1,r}x^r = \sum_{r=0}^{n-1} a_{n-1,r}x^{r+1} = \sum_{r=1}^{n} a_{n-1,r-1}x^r \tag{2.120}$$

it can be obtained

$$\begin{aligned}(\forall n \geq 2)\quad \sum_{r=0}^{n} a_{nr}x^r = A_n \sum_{r=1}^{n} a_{n-1,r-1}x^r - \\ - B_n \sum_{r=0}^{n-1} a_{n-1,r}x^r - C_n \sum_{r=0}^{n-2} a_{n-2,r}x^r.\end{aligned} \tag{2.121}$$

Coefficients a_{nr} are independent of *x*; thus, from (2.121) follows

$$\begin{aligned}&a_{n,0} = -B_n a_{n-1,0} - C_n a_{n-2,0},\\ &(r = 1,\ldots,n-2)\quad a_{nr} = A_n a_{n-1,r-1} - B_n a_{n-1,r} - C_n a_{n-2,r},\\ &a_{n,n-1} = A_n a_{n-1,n-2} - B_n a_{n-1,n-1},\\ &a_{nn} = A_n a_{n-1,n-1}.\end{aligned} \tag{2.122}$$

Procedure for calculating coefficients a_{nr} of Jacobi polynomials $Q_n^{\alpha\beta}(x)$, generalised Fourier coefficients β_n and coefficients α_r (2.19) of resultant approximation polynomial $\tilde{f}(x,\alpha)$ (2.1) is given in Algorithm 2.5.

Algorithm 2.5. Coefficients α_r in the Jacobi polynomial approximation

List of input variables: α, β, *N*, **f*, **w* // "*"denotes pointers to $f(x)$, $w(x)$
List of output variables: α_r // "//" = beginning of a comment

// Polynomial $Q_0^{\alpha\beta}(x) = 1$
  $a_{0,0} = 1$
  Calculate d_0, J_0 // Equations (2.115) and (2.116)
  $\beta_0 = J_0 / d_0$ // Equation (2.117)

// Polynomial $Q_1^{\alpha\beta}(x) = [2(\alpha+1) + (\alpha+\beta+2)(x-1)]/2$
  $a_{1,0} = (\alpha - \beta)/2$

$a_{1,1} = (\alpha + \beta + 2)/2$

Calculate d_1, J_1 // Equations (2.115) and (2.116)

$\beta_1 = (a_{1,0} J_0 + a_{1,1} J_1)/d_1$ // Equation (2.117)

// Polynomials $Q_2^{\alpha\beta}(x)$, …, $Q_{N-1}^{\alpha\beta}(x)$

for $n = 2, ..., N-1$

// Calculating coefficients a_{nr} of $Q_n^{\alpha\beta}(x)$ by using recursion (2.100)

$$A_n = \frac{(2n+\alpha+\beta-1)(2n+\alpha+\beta)}{2n(n+\alpha+\beta)}$$

$$B_n = \frac{(\alpha+\beta)(\alpha-\beta)(2n+\alpha+\beta-1)}{2n(n+\alpha+\beta)(2n+\alpha+\beta-2)}$$ // Equations (2.101)

$$C_n = \frac{(n+\alpha-1)(n+\beta-1)(2n+\alpha+\beta)}{n(n+\alpha+\beta)(2n+\alpha+\beta-2)}$$

$a_{n,0} = -B_n a_{n-1,0} - C_n a_{n-2,0}$

for $r = 1, ..., n-2$

$a_{nr} = A_n a_{n-1,r-1} - B_n a_{n-1,r} - C_n a_{n-2,r}$ // Equation (2.122)

endfor

$a_{n,n-1} = A_n a_{n-1,n-2} - B_n a_{n-1,n-1}$

$a_{nn} = A_n a_{n-1,n-1}$

Calculate d_n, J_n // Equations (2.115) and (2.116)

$$\beta_n = \sum_{r=0}^{n} a_{nr} J_r / d_n$$ // Equation (2.117)

endfor

// Calculating coefficients α_r of approximation polynomial $\tilde{f}(x,\alpha)$ (2.1)

for $r = 0, ..., N-1$

$$\alpha_r = \sum_{n=r}^{N-1} \beta_n a_{nr}$$ // Equation (2.19)

endfor

end

2.2.10 Laguerre polynomials

Polynomials $L_n(x)$ $(n = 0, 1, 2, \ldots)$ that are orthonormal with respect to the weighting function $w(x) = e^{-x}$ on the interval $[0, \infty)$ are called *Laguerre polynomials*. They satisfy orthogonality condition

$$\langle L_n, L_m \rangle = \int_0^\infty e^{-x} L_n(x) L_m(x) \mathrm{d}x = \delta_{nm} . \tag{2.123}$$

The Laguerre polynomials are given by Rodrigue's formula[7]

$$\begin{aligned} &L_0(x) = 1, \\ &(\forall n > 1) \quad L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} (e^{-x} x^n), \end{aligned} \tag{2.124}$$

or by explicit formula

$$L_n(x) = \sum_{k=0}^{n} \binom{n}{n-k} \frac{(-x)^k}{k!}. \tag{2.125}$$

The general recursion relation is

$$(\forall n \geq 1) \quad L_n(x) = \frac{2n-1-x}{n} L_{n-1}(x) - \frac{n-1}{n} L_{n-2}(x) , \tag{2.126}$$

starting with $L_0(x) = 1$.

Example 2.5. First few Laguerre polynomials are

$$\begin{aligned} L_0 &= 1, \\ L_1 &= -x + 1, \\ L_2 &= \frac{1}{2!}(x^2 - 4x + 2), \\ L_3 &= \frac{1}{3!}(-x^3 + 9x^2 - 18x + 6), \\ L_4 &= \frac{1}{4!}(x^4 - 16x^3 + 72x^2 - 96x + 24), \\ L_5 &= \frac{1}{5!}(-x^5 + 25x^4 - 200x^3 + 600x^2 - 600x + 120), \\ L_6 &= \frac{1}{6!}(x^6 - 36x^5 + 450x^4 - 2400x^3 + 5400x^2 - 4320x + 720). \end{aligned} \tag{2.127}$$

[7] The Laguerre polynomials satisfy the differential equation $xy'' + (1-x)y' + ny = 0$.

2.2.11 Generalised Laguerre polynomials

Polynomials $L_n^{(\alpha)}(x)$ ($n = 0, 1, 2, \ldots$) that are orthogonal with respect to the weighting function $w(x) = x^\alpha e^{-x}$ ($\alpha > -1$) on the interval $[0, \infty)$, are called *generalised Laguerre polynomials*. Sometimes, they are also called *associated Laguerre polynomials*. They satisfy orthogonality condition[8]

$$\langle L_n^{(\alpha)}, L_m^{(\alpha)} \rangle = \int_0^\infty x^\alpha e^{-x} L_n^{(\alpha)}(x) L_m^{(\alpha)}(x)\,\mathrm{d}x = \frac{\Gamma(n+\alpha+1)}{n!}\delta_{nm}\,. \tag{2.128}$$

The generalised Laguerre polynomials are given by Rodrigue's formula

$$\begin{aligned} &L_0^{(\alpha)}(x) = 1, \\ &(\forall n \geq 1) \quad L_n^{(\alpha)}(x) = \frac{x^{-\alpha}e^x}{n!}\frac{d^n}{dx^n}(e^{-x}x^{n+\alpha}), \end{aligned} \tag{2.129}$$

or by explicit formula

$$L_n^{(\alpha)}(x) = \sum_{k=0}^{n} \binom{n+\alpha}{n-k} \frac{(-x)^k}{k!}. \tag{2.130}$$

The general recursion relation is

$$(\forall n \geq 1) \quad L_n^{(\alpha)}(x) = \frac{2n+\alpha-1-x}{n} L_{n-1}^{(\alpha)}(x) - \frac{n+\alpha-1}{n} L_{n-2}^{(\alpha)}(x)\,, \tag{2.131}$$

starting with $L_0^{(\alpha)}(x) = 1$.

The simple Laguerre polynomials are identical to generalised one for $\alpha = 0$, i.e.

$$L_n^{(0)}(x) = L_n(x)\,. \tag{2.132}$$

Example 2.6. First few generalised Laguerre polynomials are

$$\begin{aligned} L_0^{(\alpha)} &= 1, \\ L_1^{(\alpha)} &= -x + \alpha + 1, \\ L_2^{(\alpha)} &= \frac{1}{2!}(x^2 - 2(\alpha+2)x + (\alpha+1)(\alpha+1)), \\ L_3^{(\alpha)} &= \frac{1}{3!}(-x^3 + 3(\alpha+3)x^2 - 3(\alpha+2)(\alpha+3)x + 6)x + (\alpha+1)(\alpha+2)(\alpha+3)). \end{aligned} \tag{2.133}$$

[8] *Gama function* $\Gamma(x)$ is described in Appendix A.

2.2.12 Hermite polynomials

There are two types of Hermite polynomials:

a) *physicists' Hermite polynomials*, classical polynomials in physics, where they are used mostly in analyses of the eigenstates and the quantum harmonic oscillator, and

b) *probabilists' Hermite polynomials*, classical orthogonal polynomials sequences that arise in probability and in combinatorics.

They are named in the honour of Charles Hermite.

The physicists' Hermite polynomials are orthogonal with respect to the weighting function $w(x)=e^{-x^2}$ on the interval $(-\infty,\infty)$ and standardised with condition $H_n(x)=2^n x^n+\ldots$ (leading coefficient of polynomials has value 2^n). They are given by Rodrigue's formula[9]

$$H_n(x)=(-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}\,. \tag{2.134}$$

They can be also defined by generalised Laguerre polynomials as

$$\begin{aligned}H_{2n}(x)&=(-4)^n n!\,L_n^{(-1/2)}(x^2),\\ H_{2n+1}(x)&=2(-4)^n n!\,xL_n^{(1/2)}(x^2),\end{aligned} \tag{2.135}$$

or with explicit expressions

$$\begin{aligned}H_{2n}(x)&=2^{2n}n!\sum_{r=0}^{n}(-1)^{n-r}\binom{n-1/2}{n-r}\frac{x^{2r}}{r!},\\ H_{2n+1}(x)&=2^{2n+1}n!\sum_{r=0}^{n}(-1)^{n-r}\binom{n+1/2}{n-r}\frac{x^{2r+1}}{r!}.\end{aligned} \tag{2.136}$$

The general recursion relation is

$$(\forall n\geq 1)\quad H_n(x)=2xH_{n-1}(x)-2(n-1)H_{n-2}(x)\,, \tag{2.137}$$

starting with $H_0(x)=1$.

[9] The physicists Hermite polynomials are solution of the *Hermite differential equation* $y''-2xy'+2ny=0$.

Example 2.7. First few physicists' Hermite polynomials are

$$H_0 = 1, \qquad H_6 = 2^6 x^6 - 480x^4 + 720x^2 - 120, \tag{2.138}$$
$$H_1 = 2x, \qquad H_7 = 2^7 x^7 - 1344x^5 + 3360x^3 - 1680x,$$
$$H_2 = 2^2 x^2 - 2, \qquad H_8 = 2^8 x^8 - 3584x^6 + 13440x^4 - 13440x^2 + 1680,$$
$$H_3 = 2^3 x^3 - 12x, \qquad H_9 = 2^9 x^9 - 9216x^7 + 48384x^5 - 80640x^3 + 30240x,$$
$$H_4 = 2^4 x^4 - 48x^2 + 12, \qquad H_{10} = 2^{10} x^{10} - 23040x^8 + 161280x^6$$
$$H_5 = 2^5 x^5 - 160x^3 + 120x, \qquad - 403200x^4 + 302400x^2 - 30240.$$

Due to their orthogonality, physicists' Hermite polynomials satisfy the expression

$$\langle H_n, H_m \rangle = \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) \mathrm{d}x = \begin{cases} 0, & m \neq n, \\ n!\, 2^n \sqrt{\pi}, & m = n. \end{cases} \tag{2.139}$$

Other important properties of physicists' Hermite polynomials[10]:

$$H_n'(x) = 2nH_{n-1}(x), \tag{2.140}$$

$$H_n(x+y) = \sum_{r=0}^{n} \binom{n}{r} H_r(x)\,(2y)^{n-r}. \tag{2.141}$$

The probabilists' Hermite polynomials are orthogonal with respect to the weighting function $w(x) = e^{-x^2/2}$ on the interval $(-\infty, \infty)$ and standardised with condition $H_n(x) = x^n + \ldots$ (leading coefficient of polynomials has value 1).

That convention is often preferred by probabilists because $e^{-x^2/2}/\sqrt{2\pi}$ is probability density function for the normal distribution with expected value 0 and standard deviation 1.
Probabilists' Hermite polynomials are given by Rodrigue's formula[11]

[10] Functions $\psi_n(x) = H_n(x)\sqrt{w(x)/\langle H_n(x), H_n(x)\rangle}$ generated from physicists' Hermite polynomials are known as Hermite functions. Since these functions contain square root of weighting function $\sqrt{w(x)}$ and have been scaled appropriately by $\sqrt{\langle H_n(x), H_n(x)\rangle}$, they are orthonormal. The Hermite functions satisfy differential equation $\psi_n''(x) + (2n+1-x^2)\psi_n(x) = 0$. This equation is equivalent to Schrödinger equation of a harmonic oscillator in a quantum mechanics, so these functions are eigenfunctions.

$$H_n(x) = (-1)^n e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2/2} \,. \tag{2.142}$$

The general recursion relation is

$$(\forall n \geq 1) \quad H_n(x) = xH_{n-1}(x) - (n-1)H_{n-2}(x) \,, \tag{2.143}$$

starting with $H_0(x) = 1$.

Example 2.8. First few probabilists' Hermite polynomials are

$$\begin{aligned}
&H_0 = 1, && H_6 = x^6 - 15x^4 + 45x^2 - 15,\\
&H_1 = x, && H_7 = x^7 - 21x^5 + 105x^3 - 105x,\\
&H_2 = x^2 - 1, && H_8 = x^8 - 28x^6 + 210x^4 - 420x^2 + 105,\\
&H_3 = x^3 - 3x, && H_9 = x^9 - 36x^7 + 378x^5 - 1260x^3 + 945x,\\
&H_4 = x^4 - 6x^2 + 3, && H_{10} = x^{10} - 45x^8 + 630x^6 - 3150x^4 + 4725x^2 - 945.\\
&H_5 = x^5 - 10x^3 + 15x, &&
\end{aligned} \tag{2.144}$$

Due to their orthogonality, probabilists' Hermite polynomials satisfy the expression

$$\langle H_n, H_m \rangle = \int_{-\infty}^{\infty} e^{-x^2/2} H_n(x) H_m(x) \mathrm{d}x = \begin{cases} 0, & m \neq n, \\ n!\sqrt{2\pi}, & m = n. \end{cases} \tag{2.145}$$

Other properties of probabilists' Hermite polynomials:

$$H_n'(x) = nH_{n-1}(x) \,, \tag{2.146}$$

$$H_n(x+y) = \sum_{r=0}^{n} \binom{n}{r} x^r H_{n-r}(y) \,. \tag{2.147}$$

[11] The probabilists' Hermite polynomials are also solution of differential equation $\frac{\mathrm{d}}{\mathrm{d}x}\left(e^{-x^2/2} \frac{\mathrm{d}}{\mathrm{d}x} y\right) + n\, e^{-x^2/2} y = 0$, where n is a constant, with the boundary condition that y should be polynomially bounded to infinity. With that boundary condition, the equation has a solution only if n is a positive integer and is uniquely given by $y(x) = H_n(x)$.

Generalisation of Hermite polynomials. The probabilistics' Hermite polynomials defined above are orthogonal with respect to the standard normal probability distribution, whose density function $e^{-x^2/2}/\sqrt{2\pi}$, has expected value 0 and variance $\alpha = 1$. Generalised Hermite polynomials can be defined as polynomials $H_n^{[\alpha]}(x)$ of arbitrary variance α. These are orthogonal with respect to the normal probability distribution whose density function is

$$w(x) = \frac{e^{-x^2/(2\alpha)}}{\sqrt{2\pi\alpha}}. \tag{2.148}$$

They are given by

$$H_n^{[\alpha]}(x) = \frac{1}{\alpha^{n/2}} H_n^{[1]}\left(\frac{x}{\sqrt{\alpha}}\right), \tag{2.149}$$

where $H_n^{[1]}(x) \equiv H_n(x)$ are probabilists' Hermite polynomials. The physicists' Hermite polynomials are

$$H_n^{[1/2]}(x) = 2^{n/2} H_n^{[1]}(\sqrt{2}x). \tag{2.150}$$

The important properties of Hermite polynomials in generalised form are

$$H_n'^{[\alpha]}(x) = 2nH_{n-1}^{[\alpha]}(x), \tag{2.151}$$

$$H_{n-1}^{[\alpha+\beta]}(x+y) = \sum_{r=0}^{n} \binom{n}{r} H_r^{[\alpha]}(x) H_{n-r}^{[\beta]}(y). \tag{2.152}$$

Hermite polynomials with negative variance are denoted as $H_n^{[-\alpha]}(x)$. For $\alpha > 0$, the coefficients of $H_n^{[-\alpha]}(x)$ are just the absolute values of the corresponding coefficients of $H_n^{[\alpha]}(x)$. These arise as a moment of normal probability distributions. The n^{th} moment of the normal distribution with expected value μ and variance σ^2 is

$$E(X^n) = H_n^{[-\sigma^2]}(\mu), \tag{2.153}$$

where X is a random variable with the specified normal distribution.

2.3 MULTIPLE POWER SERIES

The idea of least-squares power series expansion for a function of single variable x can be extended to the case of functions of two or more variables: x_1, x_2, …, x_M. For example, function $f(x) = f(x_1, x_2)$ of two variables x_1 and x_2 can be approximated by the polynomial

$$\tilde{f}(x,\alpha) = \sum_{r_1=0}^{N_1-1} \sum_{r_2=0}^{N_2-1} \alpha_{r_1 r_2} x_1^{r_1} x_2^{r_2} , \tag{2.154}$$

where N_1 is constant, while N_2 can be either constant or a function of $N_2(r_1)$ (e.g. $N_2(r_1) = N_1 - r_1$). Coefficients $\alpha_{r_1 r_2}$ can be determined by the least-squares method.

By analogy to (1.81), the mean square error is defined on a two dimensional domain Ω as

$$\begin{aligned} E_{\mathrm{ms}}(\alpha) &= \frac{1}{\int_\Omega \mathrm{d}\Omega(x)} \int_\Omega w(x)[f(x) - \tilde{f}(x,\alpha)]^2 \, \mathrm{d}\Omega(x) \\ &= \frac{1}{\int_\Omega \mathrm{d}\Omega(x)} \int_\Omega w(x) \left(f(x) - \sum_{r_1=0}^{N_1-1} \sum_{r_2=0}^{N_2-1} \alpha_{r_1 r_2} x_1^{r_1} x_2^{r_2} \right)^2 \mathrm{d}\Omega(x) . \end{aligned} \tag{2.155}$$

From the condition of extreme in respect to the coefficients $\alpha_{r_1 r_2}$ it follows

$$\begin{gathered} (\forall (n_1, n_2) \,|\, n_1 = 0, ..., N_1 - 1;\ n_2 = 0, ..., N_2(n_1) - 1) \\ \frac{\partial E_{\mathrm{ms}}(\alpha)}{\partial \alpha_{n_1 n_2}} = 0 \Rightarrow \int_\Omega w(x) \left(f(x) - \sum_{r_1=0}^{N_1-1} \sum_{r_2=0}^{N_2-1} \alpha_{r_1 r_2} x_1^{r_1} x_2^{r_2} \right) x_1^{n_1} x_2^{n_2} \, \mathrm{d}\Omega(x) = 0, \end{gathered} \tag{2.156}$$

or

$$\begin{gathered} (\forall (n_1, n_2) \,|\, n_1 = 0, ..., N_1 - 1;\ n_2 = 0, ..., N_2(n_1) - 1) \\ \sum_{r_1=0}^{N_1-1} \sum_{r_2=0}^{N_2-1} \alpha_{r_1 r_2} \int_\Omega w(x)\, x_1^{r_1+n_1} x_2^{r_2+n_2} \, \mathrm{d}\Omega(x) = \int_\Omega w(x)\, f(x)\, x_1^{n_1} x_2^{n_2} \, \mathrm{d}\Omega(x) . \end{gathered} \tag{2.157}$$

This linear equation system can be expressed in the terms of the weighted inner product on a continuous domain Ω:

$$\langle\langle \phi,\psi \rangle\rangle = \int_{\Omega} w(x)\,\phi(x)\,\psi(x)\,\mathrm{d}\Omega(x) \tag{2.158}$$

as[12]

$$\begin{gathered}(\forall (n_1,n_2)\,|\, n_1 = 0,\ldots,N_1-1;\; n_2 = 0,\ldots,N_1(n_1)-1)\\ \sum_{r_1=0}^{N_1-1}\sum_{r_2=0}^{N_2-1}\langle\langle x_1^{r_1}x_2^{r_2}, x_1^{n_1}x_2^{n_2}\rangle\rangle\,\alpha_{r_1r_2} = \langle\langle f, x_1^{n_1}x_1^{n_2}\rangle\rangle\,.\end{gathered} \tag{2.159}$$

Solution of this linear equation system are coefficients $\alpha_{r_1r_2}$.

As it is already outlined in Chapter 1.3.2, the linear equation system (2.159) can be ill-conditioned and its numerical solution (coefficients $\alpha_{r_1r_2}$) can have intolerable error.

In general, monomials $x_1^{r_1}x_2^{r_2}$ can be expressed as a sum of polynomials

$$x_1^{r_1}x_2^{r_2} = \sum_{n_1=0}^{r_1}\sum_{n_2=0}^{r_2}\gamma_{n_1n_2}\,p_{n_1}^{[1]}(x_1)\,p_{n_2}^{[2]}(x_2)\,. \tag{2.160}$$

Therefore, function $f(x)$ that can be expanded into series of monomials $x_1^{r_1}x_2^{r_2}$, can also be expand into the series of polynomials

$$f(x,\beta) = \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\beta_{n_1n_2}\,p_{n_1}^{[1]}(x_1)\,p_{n_2}^{[2]}(x_2)\,. \tag{2.161}$$

To avoid solving the linear equation system (2.159), the used polynomials

$$\begin{aligned}p_{n_1}^{[1]}(x_1) &= \sum_{r_1=0}^{n_1} a_{n_1r_1}^{[1]}x_1^{r_1} = a_{n_1n_1}^{[1]}x_1^{n_1} + a_{n_1,n_1-1}^{[1]}x_1^{n_1-1} + \ldots + a_{n_1,1}^{[1]}x_1 + a_{n_1,0}^{[1]},\\ p_{n_2}^{[2]}(x_2) &= \sum_{r_2=0}^{n_2} a_{n_2r_2}^{[2]}x_2^{r_2} = a_{n_2n_2}^{[2]}x_2^{n_2} + a_{n_2,n_2-1}^{[2]}x_2^{n_2-1} + \ldots + a_{n_2,1}^{[2]}x_2 + a_{n_2,0}^{[2]},\end{aligned} \tag{2.162}$$

have to be orthogonal, i.e., their coefficients $a_{n_1r_1}^{[1]}$ and $a_{n_2r_2}^{[2]}$ have to be determined by the orthogonality condition

---

[12] Double brackets $\langle\langle \ldots \rangle\rangle$ are used to denote the weighted inner product on a two--dimensional domain and to distinct it from the inner product on the interval.

$$\langle\langle p_{n_1}^{[1]} p_{n_2}^{[2]}, p_{m_1}^{[1]} p_{m_2}^{[2]} \rangle\rangle = \tag{2.163}$$

$$= \int_\Omega w(x) p_{n_1}^{[1]}(x_1) p_{n_2}^{[2]}(x_2) p_{m_1}^{[1]}(x_1) p_{m_2}^{[2]}(x_2)\, \mathrm{d}\Omega(x) \begin{cases} = 0, & (m_1, m_2) \neq (n_1, n_2), \\ \neq 0, & (m_1, m_2) = (n_1, n_2), \end{cases}$$

with respect to some weighting function $w(x) = w(x(x_1, x_2))$ on a domain Ω.

Herein, an integral over a domain Ω can be expressed in the form

$$\int_\Omega (...)\, \mathrm{d}\Omega(x) = \int_{a_1}^{b_1} \int_{a_2}^{b_2} (...)\, \mathrm{d}x_1\, \mathrm{d}x_2 \,, \tag{2.164}$$

where a_1 and b_1 are constants, while a_2 and b_2 can be either constants (on rectangle domain Ω, Fig. 2.2.*a*) or functions $a_2 = a_2(x_1)$ and $b_2 = b_2(x_1)$ (if domain Ω has some other shape, Fig.2.2.*b*).

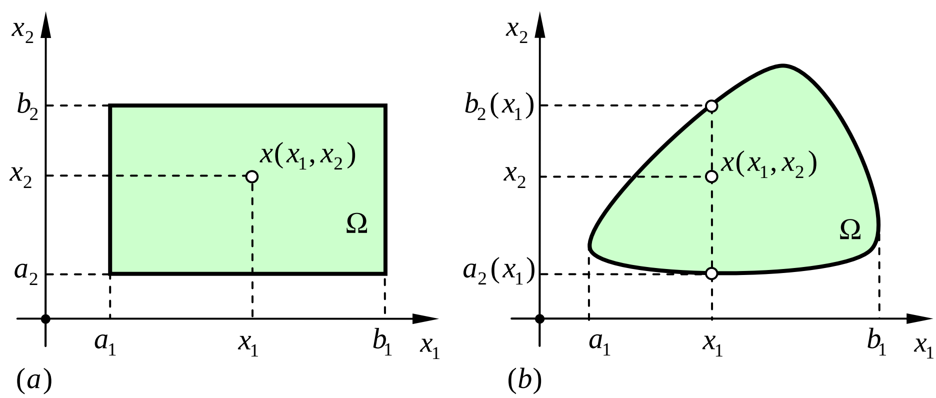

Fig. 2.2. *Independent* (*a*) *and dependent* (*b*) *intervals in the 2D space*

In the special case, when intervals $[a_1, b_1]$ and $[a_2, b_2]$ are both constant (Fig. 2.2.*a*), the integral over domain Ω can be divided into the two integrals

$$\int_\Omega A(x_1) B(x_2)\, \mathrm{d}\Omega(x) = \left(\int_{a_1}^{b_1} A(x_1)\, \mathrm{d}x_1 \right) \left(\int_{a_2}^{b_2} B(x_2)\, \mathrm{d}x_2 \right). \tag{2.165}$$

In a such case

$$\langle\langle p_{n_1}^{[1]} p_{n_2}^{[2]}, p_{m_1}^{[1]} p_{m_2}^{[2]} \rangle\rangle = \langle p_{n_1}^{[1]}, p_{m_1}^{[1]} \rangle \langle p_{n_2}^{[2]}, p_{m_2}^{[2]} \rangle \,, \tag{2.166}$$

while the orthogonality condition (2.163) is divided into two independent ones

$$\begin{aligned} \langle p_{n_1}^{[1]}, p_{m_1}^{[1]} \rangle &= \int_{a_1}^{b_1} w^{[1]}(x_1) p_{n_1}^{[1]}(x_1) p_{m_1}^{[1]}(x_1)\,\mathrm{d}x_1 \quad \begin{cases} = 0, & m_1 \neq n_1, \\ \neq 0, & m_1 = n_1, \end{cases} \\ \langle p_{n_2}^{[2]}, p_{m_2}^{[2]} \rangle &= \int_{a_2}^{b_2} w^{[2]}(x_2) p_{n_2}^{[2]}(x_2) p_{m_2}^{[2]}(x_2)\,\mathrm{d}x_2 \quad \begin{cases} = 0, & m_2 \neq n_2, \\ \neq 0, & m_2 = n_2, \end{cases} \end{aligned} \tag{2.167}$$

with respect to the weighting functions $w^{[1]}(x_1)$ and $w^{[2]}(x_2)$ on intervals $[a_1,b_1]$ and $[a_2,b_2]$ respectively. The generalised Fourier coefficients are then

$$\begin{aligned} \beta_{n_1 n_2} &= \frac{\langle\langle f, p_{n_1}^{[1]} p_{n_2}^{[2]} \rangle\rangle}{\langle p_{n_1}^{[1]}, p_{n_1}^{[1]} \rangle \langle p_{n_2}^{[2]}, p_{n_2}^{[2]} \rangle} = \\ &= \frac{\int_{a_1}^{b_1}\int_{a_2}^{b_2} w^{[1]}(x_1) w^{[2]}(x_2) f(x_1,x_2)\, p_{n_1}^{[1]}(x_1) p_{n_2}^{[2]}(x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2}{\left(\int_{a_1}^{b_1} w^{[1]}(x_1)[p_{n_1}^{[1]}(x_1)]^2\,\mathrm{d}x_1\right)\left(\int_{a_2}^{b_2} w^{[2]}(x_2)[p_{n_2}^{[2]}(x_2)]^2\,\mathrm{d}x_2\right)}. \end{aligned} \tag{2.168}$$

The described approximation procedure can be generalised to *triple power series*, etc.

2.3.1 Zernike polynomials

The polynomials that are orthogonal on the unit disk with respect to the radial distance as a weighting function, are known as the Zernike polynomials[13]. They are defined in a polar coordinate system $\rho - \varphi$ (Fig. 2.3), where φ is azimuthal angle, and ρ is normalised radial distance. There are even and odd Zernike polynomials. The even Zernike polynomials are defined as

$$Z_n^m(\rho,\varphi) = R_n^m(\rho)\cos m\varphi\,, \tag{2.169}$$

and the odd Zernike polynomials as

$$Z_n^{-m}(\rho,\varphi) = R_n^m(\rho)\sin m\varphi\,, \tag{2.170}$$

[13] Zernike polynomials are named after Fritz Zernike. They are used in precision optical manufacturing to characterise high order errors. In optometry and ophthalmology they are used to describe aberrations of the cornea or lens from an ideal spherical shape, which results in refraction errors. They can be used to effectively cancel out atmospheric distortion. Obvious applications for this are IR or visual astronomy, and spy satellites. For example, the term Z_2^0 is called „de-focusing“. By coupling the output from this term to a control system, an automatic focus can be implemented.

where m and $n \ge m \ge 0$ are nonnegative integers, φ is azimuthal angle $0 \le \varphi \le 2\pi$, and ρ is normalised radial distance $0 \le \rho \le 1$. The radial polynomials $R_n^m(\rho)$ are defined as

$$R_n^m(\rho) = \sum_{k=0}^{(n-m)/2} \frac{(-1)^k (n-k)!}{k!((n+m)/2-k)!((n-m)/2-k)!} \rho^{n-2k}, \qquad (2.171)$$

when $(n-m)/2$ is integer, and as $R_n^m(\rho) = 0$ for odd $n-m$.

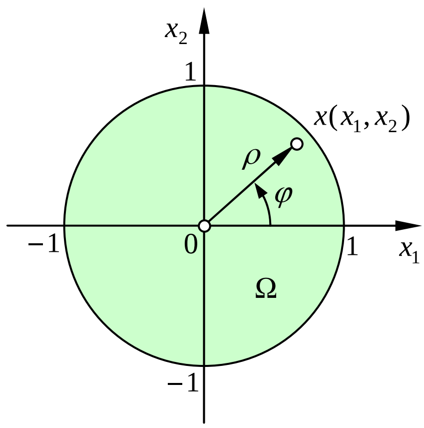

Fig. 2.3. *Unit disk and coordinate systems*

In the terms of Jacobi polynomials

$$R_n^m(\rho) = (-1)^{(n-m)/2} \rho^m Q_{(n-m)/2}^{m,0}(1-2\rho^2) \quad (\text{even } n-m). \qquad (2.172)$$

Zernike polynomials are standardised with the condition that $R_n^m(1) = 1$ when $(n-m)/2$ is integer, otherwise $R_n^m(1) = 0$.

Example 2.9. First few nonzero radial polynomials are

$$\begin{aligned}
&R_0^0 = 1, \\
&R_1^1 = \rho, \\
&R_2^0 = 2\rho^2 - 1, \quad R_2^2 = \rho^2, \\
&R_3^1 = 3\rho^3 - 2\rho, \quad R_3^3 = \rho^3, \\
&R_4^0 = 6\rho^4 - 6\rho^2 + 1, \quad R_4^2 = 4\rho^4 - 3\rho^2, \quad R_4^4 = \rho^4.
\end{aligned} \qquad (2.173)$$

The radial polynomials satisfy the orthogonality relation

$$\int_0^1 \rho\, R_n^m(\rho) R_{n_1}^m(\rho)\,\mathrm{d}\rho = \begin{cases} 0, & n \neq n_1, \\ \dfrac{R_n^m(1)}{2(n+1)}, & n = n_1. \end{cases} \tag{2.174}$$

The angular part of Zernike polynomials satisfy the orthogonality relations

$$\begin{aligned} &\int_0^{2\pi} \sin n\varphi \sin m\varphi \,\mathrm{d}\varphi = \begin{cases} 0, & n \neq m, \\ \pi, & n = m, \end{cases} \\ &\int_0^{2\pi} \cos n\varphi \cos m\varphi \,\mathrm{d}\varphi = \begin{cases} 0, & n \neq m, \\ \pi, & n = m, \end{cases} \\ &\int_0^{2\pi} \sin n\varphi \cos m\varphi \,\mathrm{d}\varphi = 0. \end{aligned} \tag{2.175}$$

Zernike polynomials $Z_n^m(\rho,\varphi)$ can be converted to the rectangular form $Z_n^m(x_1,x_2)$ by using the following coordinate transformations and trigonometric identities

$$\begin{aligned} &x_1 = \rho\cos\varphi, \\ &x_2 = \rho\sin\varphi, \\ &\rho^2 = x_1^2 + x_2^2, \\ &\cos m\varphi = 2\cos[(m-1)\varphi]\cos\varphi - \cos[(m-2)\varphi], \\ &\sin m\varphi = 2\sin[(m-1)\varphi]\cos\varphi - \sin[(m-2)\varphi]. \end{aligned} \tag{2.176}$$

Example 2.10. First few nonzero Zernike polynomials are

$$\begin{aligned} &Z_0^0 = 1, \\ &Z_1^1 = x_1, && Z_1^{-1} = x_2, \\ &Z_2^0 = 2x_1^2 + 2x_2^2 - 1, \\ &Z_2^2 = x_1^2 - x_2^2, && Z_2^{-2} = 2x_1x_2, \\ &Z_3^1 = 3x_1^3 + 3x_1x_2^2 - 2x_1, && Z_3^{-1} = 3x_2^3 + 3x_1^2x_2 - 2x_2, \\ &Z_3^3 = x_1^3 - 3x_1x_2^2, && Z_3^{-3} = -x_2^3 + 3x_1^2x^2. \end{aligned} \tag{2.177}$$

Zernike polynomials have simple rotational symmetry that distinguishes them from the other sets of orthogonal polynomials. This is illustrated on Fig. 2.4 by coloured areas on the unit disks. The polynomials Z_n^m have positive values on green areas, negative values on red areas and the zero value on black null-lines.

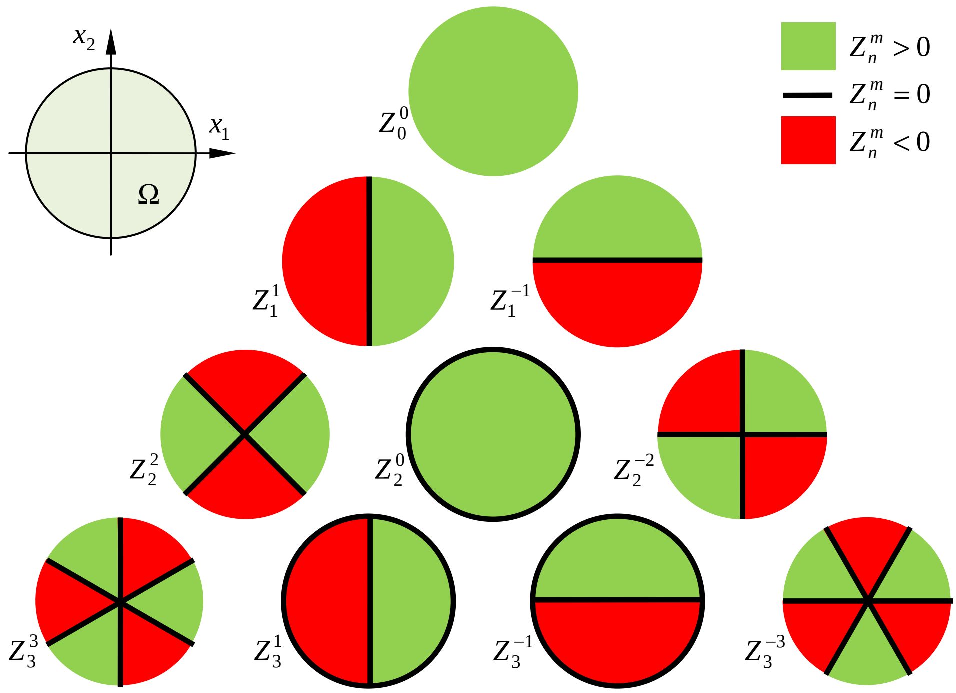

Fig. 2.4. *Null-lines of Zernike polynomials*

Expansion with Zernike polynomials

$$f(x) = \sum_{m=0}^{\infty} \sum_{n=m}^{\infty} (a_n^m Z_n^{-m} + b_n^m Z_n^m) \tag{2.178}$$

is given by generalised Fourier coefficients

$$\begin{aligned} a_n^m &= \frac{n+1}{\varepsilon_{mn}^2 \pi} \int_0^1 \int_0^{2\pi} f(\rho,\varphi) Z_n^{-m} \rho \, \mathrm{d}\varphi \, \mathrm{d}\rho, \\ b_n^m &= \frac{n+1}{\varepsilon_{mn}^2 \pi} \int_0^1 \int_0^{2\pi} f(\rho,\varphi) Z_n^{m} \rho \, \mathrm{d}\varphi \, \mathrm{d}\rho, \end{aligned} \tag{2.179}$$

where

$$\varepsilon_{mn} = \begin{cases} 1/\sqrt{2}, & \text{for } m = 0, n \neq 0, \\ 1, & \text{otherwise.} \end{cases} \tag{2.180}$$

2.4 APPROXIMATION ON A DISCRETE DOMAIN

Consider that approximated function $f(x)$ is defined by a table, i.e. by the sampling values $f^k = f(\xi^k)$ in the finite set of K distinct sampling points ξ^k. In a such case, function $f(x)$ can be approximated by a polynomial

$$\tilde{f}(x,\alpha) = \sum_{r=0}^{N-1} \alpha_r x^r \,, \quad N \le K \,, \tag{2.181}$$

whose coefficients α_r can be determined by the least-squares method. The difference between polynomials (2.1) and (2.181) is in the fact that in the discrete approximation only up to K coefficients α_r can be determined by K sampling values $f^k = f(\xi^k)$; thus, in the discrete approximation, the degree of the polynomial $\tilde{f}(x,\alpha)$ can only be lesser than the number of distinct sampling points.

By analogy to (1.88), a mean square error is defined as

$$\begin{aligned} E_{\mathrm{ms}}(\alpha) &= \frac{1}{K}\sum_{k=1}^{K} w^k [f^k - \tilde{f}(\xi^k,\alpha)]^2 \\ &= \frac{1}{K}\sum_{k=1}^{K} w^k \left[f^k - \sum_{r=0}^{N-1} \alpha_r (\xi^k)^r \right]^2 . \end{aligned} \tag{2.182}$$

From the condition of extreme in the respect to coefficients α_r it follows

$$\begin{aligned} &(\forall n = 0,\ldots, N-1 \,|\, N \le K) \\ &\frac{\partial E_{\mathrm{ms}}(\alpha)}{\partial \alpha_n} = 0 \Rightarrow \sum_{k=1}^{K} w^k \left[f^k - \sum_{r=0}^{N-1} \alpha_r \cdot (\xi^k)^r \right] (\xi^k)^n = 0, \end{aligned} \tag{2.183}$$

or

$$\begin{aligned} &(\forall n = 0,\ldots, N-1 \,|\, N \le K) \\ &\sum_{r=0}^{N-1} \alpha_r \sum_{k=1}^{K} w^k \cdot (\xi^k)^{r+n} = \sum_{k=1}^{K} w^k f^k \cdot (\xi^k)^n . \end{aligned} \tag{2.184}$$

This linear equation system can be expressed in the terms of weighted inner product

$$\langle \phi,\psi \rangle = \sum_{k=1}^{K} w^k \, \phi(\xi^k)\, \psi(\xi^k) \tag{2.185}$$

as

$$(\forall n = 0, ..., N-1) \ \sum_{r=0}^{N-1} \alpha_r \langle x^r, x^n \rangle = \langle f, x^n \rangle , \qquad N \le K . \tag{2.186}$$

Solution of this linear equation system are coefficients α_r. This linear equation system differs from system (2.6) in the definition of inner product and in a limited number of equations $N \le K$. It is also usually ill-conditioned (as described in the Chapter 1.3.2), so its numerical solution (coefficients α_r) can have intolerable error.

To avoid solving the linear equation system (2.186), function $f(x)$ can be expanded into finite series

$$\tilde{f}(x,\beta) = \sum_{n=0}^{N-1} \beta_n p_n(x) , \qquad N \le K , \tag{2.187}$$

of orthogonal polynomials $p_n(x)$ with degree n not greater than $K-1$. The coefficients a_{nr} of polynomials $p_n(x)$ (2.8) are determined by the orthogonality condition

$$\langle p_n, p_m \rangle = \sum_{k=1}^{K} w^k p_n(\xi^k) p_m(\xi^k) \begin{cases} = 0, & m \ne n, \\ \ne 0, & m = n, \end{cases} \tag{2.188}$$

with respect to the given set of weighting coefficients w^k.

Approximation with a finite series $\tilde{f}(x,\beta)$ (2.187) defined as a partial sum of the first N elements containing orthogonal polynomials $p_n(x)$, with the degrees n no greater than $N-1$, is a *polynomial least-squares approximation* of $f(x)$. Therefore, coefficients β_n are generalised Fourier coefficients that can be obtained by substituting $\phi_n(x) = p_n(x)$ into (1.74) as

$$\beta_n = \frac{\langle f, p_n \rangle}{\langle p_n, p_n \rangle} = \frac{\sum_{k=1}^{K} w^k f^k p_n(\xi^k)}{\sum_{k=1}^{K} w^k [p_n(\xi^k)]^2} . \tag{2.189}$$

Although the generalised Fourier coefficients β_n of approximation function $\tilde{f}(x,\beta)$ (2.187), written in the terms of inner products, have the form equal to that in a continuous case (2.10), there is one crucial difference. By the K values

$f^k = f(\xi^k)$ of function $f(x)$ in K distinct sampling points ξ^k it can be determined up to K generalised Fourier coefficients β_n $(n = 0, 1, ..., K-1)$. Coefficients β_n $(n \geq K)$ are assumed to be zero.

Therefore, approximation function $\tilde{f}(x, \beta)$ is restricted to the first K summands $\beta_n p_n$ (i.e. $n = 0, 1, ..., N-1$ and $N \leq K$). Using all of the first K summands $\beta_n p_n$ turns approximation into interpolation, in which the value of the function and its approximation equals in all sampling points ξ^k (i.e. $\tilde{f}(\xi^k, \beta) = f^k$). This is described in Chapter 6.

A special class of orthogonal polynomials are *orthonormal polynomials*. If the weighting coefficients w^k are positive, then the weighted inner product

$$\langle p_n, p_n \rangle = \sum_{k=1}^{K} w^k [p_n(\xi^k)]^2 \tag{2.190}$$

is also positive and the set of orthogonal polynomials $\{p_n(x)\}$ can be *normalised* by dividing each polynomial $p_n(x)$ with its *norm* $\|p_n\| = \sqrt{\langle p_n, p_n \rangle}$ (2.13) [3].

The *normalised* set of polynomials $\overline{p}_n(x) = p_n(x)/\|p_n\|$ is said to be *orthonormal* with respect to the weighting coefficients w^k on a finite set of distinct sampling points. These polynomials have properties $\langle \overline{p}_n, \overline{p}_m \rangle = \delta_{nm}$, $\|\overline{p}_n\| = \sqrt{\langle \overline{p}_n, \overline{p}_n \rangle} = 1$, as in a continuous case.

Hence, if function $f(x)$ is expanded into series of orthonormal polynomials

$$\tilde{f}(x, \overline{\beta}) = \sum_{n=0}^{N-1} \overline{\beta}_n \overline{p}_n(x), \quad N \leq K, \tag{2.191}$$

the corresponding generalised Fourier coefficients are

$$\overline{\beta}_n = \langle f, \overline{p}_n \rangle = \sum_{k=1}^{K} w^k f^k \overline{p}_n(\xi^k). \tag{2.192}$$

The form of the approximation function $\tilde{f}(x, \beta)$ (2.187) is not convenient for a numerical manipulation, but it can be expressed in a more suitable form as $\tilde{f}(x, \alpha)$ (2.1). Coefficients α_r in $\tilde{f}(x, \alpha)$ can be calculated from coefficients β_n by using equation (2.19).

2.5 ORTHOGONAL POLYNOMIALS ON A DISCRETE DOMAIN

For any set of positive weighting coefficients w^k, defined on the arbitrary set of K distinct sampling points ξ^k, exists a corresponding set of K orthogonal polynomials $\{p_n(x)\}$ $(n = 0, 1, ..., K-1)$, which satisfies the orthogonality relationship (2.188) [6, 7].

Therefore, there are many polynomial family sets orthogonal on different sets of weighting coefficients w^k and sampling points ξ^k on a discrete interval. The most important ones are *Gram* and *Chebyshev polynomials*. Due to their importance, all of these polynomials and related algorithms are described in Chapters 2. and 4. as it is listed in Table 2.2.

Table 2.2. Orthogonal polynomials and rational functions on a discrete domain

Name	Symbol	Interval	K sampling points	Weighting coefficients	Chapter
Gram polynomials[14]	$P_n^K(x)$	$[-1,1]$	equidistant on x	1	2.5.3
Chebyshev polynomials of first kind	$T_n(x)$	$[-1,1]$	roots of $T_K(x)$	1	4.1.7
			extremes of $T_K(x)$	$\frac{1}{2}, 1, ..., 1, \frac{1}{2}$	4.1.8
Shifted Chebyshev polynomials	$T_n^*(x)$	$[0,1]$	roots of $T_K^*(x)$	1	4.2.2
			extremes of $T_K^*(x)$	$\frac{1}{2}, 1, ..., 1, \frac{1}{2}$	4.2.2
Chebyshev rational functions	$R_n(x)$	$[0,\infty)$	roots of $R_K(x)$	1	4.5.6
			extremes of $R_K(x)$	$\frac{1}{2}, 1, ..., 1, \frac{1}{2}$	4.5.7

[14] Polynomials $P_n^K(x)$ $(n = 0, 1, 2, ..., K-1)$ described in Chapter 2.5.3, which are orthogonal with respect to the weighting coefficients $w^k = 1$ on the K sampling points equally spaced on the interval $[-1,1]$, are called either *Gram polynomials* or *Chebyshev polynomials* [9, 10], although the later name is usually reserved for polynomials described in Chapter 4.

In addition, in Chapters 2.5.1 and 2.5.2 two general algorithms are presented for generating polynomials orthogonal with respect to an arbitrary set of positive weighted coefficients w^k defined on an arbitrary set of sampling points ξ^k. By analogy to a continuous case, these two algorithms are based on different approaches, but they give the same results.

2.5.1 Generating orthogonal polynomials on a discrete domain

For any set of positive and finite weighting coefficients w^k, defined on the particular set of sampling points ξ^k, there exists a corresponding set of orthogonal polynomials. Let these orthogonal polynomials $p_n(x)$ be standardised by condition $p_n(x) = x^n + ...$ (the leading coefficient of each polynomial has value 1) and defined by using equation (2.21). In each sampling point ξ^k it is

$$p_n(\xi^k) = (\xi^k)^n - \sum_{m=0}^{n-1} \gamma_{nm} p_m(\xi^k) , \quad n \geq 1 . \tag{2.193}$$

To find coefficients γ_{nm}, both sides of that equation can be multiplied by $w^k p_r(\xi^k)$ and summed over $k = 1, 2, ..., K$:

$$\begin{aligned} &\sum_{k=1}^{K} w^k p_r(\xi^k) p_n(\xi^k) = \\ &\qquad = \sum_{k=1}^{K} w^k p_r(\xi^k) (\xi^k)^n - \sum_{m=0}^{n-1} \gamma_{nm} \sum_{k=1}^{K} w^k p_r(\xi^k) p_m(\xi^k) . \end{aligned} \tag{2.194}$$

This can also be written in the terms of weighted inner products by equation (2.23). Due to the presumed orthogonality condition (2.188) and by analogy to continuous case, from equation (2.23) can be obtained

$$\gamma_{nm} = \frac{\langle p_m, x^n \rangle}{\langle p_m, p_m \rangle} = \frac{\langle p_m, x^n \rangle}{\langle p_m, x^m \rangle} , \quad m = 0, ..., n-1 . \tag{2.195}$$

The difference between this equation and equation (2.26) consists only in the definition of inner products.

For the calculation of the inner products $\langle p_m, x^n \rangle$ and $\langle p_m, x^m \rangle$ it is necessary to determine coefficients a_{nr} of the orthogonal polynomials $p_n(x)$ (2.8). For that purpose, already obtained expression (2.30) can be used.

By substituting $p_n(x)$ (2.8) into inner products it can be obtained

$$\begin{aligned} \langle p_m, x^n \rangle &= \sum_{r=0}^{m} a_{mr} \langle x^r, x^n \rangle = \sum_{r=0}^{m} a_{mr} \sum_{k=1}^{K} w^k \cdot (\xi^k)^{r+n}, \\ \langle f, p_n \rangle &= \sum_{r=0}^{n} a_{nr} \langle f, x^r \rangle = \sum_{r=0}^{n} a_{nr} \sum_{k=1}^{K} w^k f^k \cdot (\xi^k)^r. \end{aligned} \tag{2.196}$$

To apply developed formulas, it is convenient to introduce auxiliary variables

$$\begin{aligned} I_r^* &= \sum_{k=1}^{K} w^k \cdot (\xi^k)^r, \\ J_r^* &= \sum_{k=1}^{K} w^k f^k \cdot (\xi^k)^r. \end{aligned} \tag{2.197}$$

By analogy to equations (2.32) and (2.33) it can be obtained

$$\begin{aligned} d_n^* &= \langle p_n, p_n \rangle = \langle p_n, x^n \rangle = \sum_{r=0}^{n} a_{nr} I_{r+n}^*, \\ \gamma_{nm} &= \frac{\langle p_m, x^n \rangle}{\langle p_m, p_m \rangle} = \frac{1}{d_m^*} \sum_{r=0}^{m} a_{mr} I_{r+n}^*, \quad m = 0, ..., n-1, \\ \beta_n &= \frac{\langle f, p_n \rangle}{\langle p_n, p_n \rangle} = \frac{1}{d_n^*} \sum_{r=0}^{n} a_{nr} J_r^*. \end{aligned} \tag{2.198}$$

Complete procedure for determining coefficients a_{nr} of orthogonal polynomials $p_n(x)$, coefficients β_n and coefficients α_r (2.19) is given in Algorithm 2.6. Obtained coefficients α_r define resultant approximation polynomial $\tilde{f}(x,\alpha)$ (2.1) in the form that is the most suitable form for further numerical manipulation.

Algorithm 2.6. Coefficients α_r for the orthogonal polynomial approximation on a discrete domain – method 1

List of input variables: N, K, w^k, f^k, ξ^k

List of output variables: α_r

// Polynomial $p_0(x) = 1$

$a_{0,0} = 1$

Calculate_and_store_sums I_0^*, J_0^* // Equation (2.197)

$d_0^* = I_0^*$; $\beta_0 = J_0^* / d_0^*$

// Polynomials $p_1(x), \ldots, p_{N-1}(x)$

for $n = 1, \ldots, N-1$

Calculate_and_store_sums I_{2n-1}^*, I_{2n}^*, J_n^* // Equation (2.197)

// Expansion of x^n into series of polynomials $p_0(x), \ldots, p_n(x)$ (2.20)

for $m = 0, \ldots, n-1$

$$\gamma_{nm} = \frac{1}{d_m^*} \sum_{r=0}^{m} a_{mr} I_{r+n}^*$$ // Equation (2.198)

endfor

// Coefficients a_{nr} of orthogonal polynomial $p_n(x)$ (2.8)

for $r = 0, \ldots, n-1$

$$a_{nr} = -\sum_{m=r}^{n-1} \gamma_{nm} a_{mr}$$ // Equation (2.130)

endfor

$a_{nn} = 1$

$d_n^* = \sum_{r=0}^{n} a_{nr} I_{r+n}^*$ // $d_n^* = \langle p_n, p_n \rangle$ (2.198)

$\beta_n = \sum_{r=0}^{n} a_{nr} J_r^* / d_n^*$ // Generalised Fourier coefficients (2.198)

endfor

// Calculating coefficients α_r of approximation polynomial $\tilde{f}(x, \alpha)$ (2.1)

for $r = 0, \ldots, N-1$

$\alpha_r = \sum_{n=r}^{N-1} \beta_n a_{nr}$ // Equation (2.19)

endfor

end

2.5.2 Generating orthogonal polynomials on a discrete domain by recursion

A more convenient and efficient method for generating orthogonal polynomials $p_n(x)$ is the use of recurrence relation

$$
\begin{aligned}
&p_0(x) = 1\,, \\
&p_1(x) = (x - b_1)\,, \\
&p_n(x) = (x - b_n)\,p_{n-1}(x) - c_{n-1}p_{n-2}(x)\,, \quad n = 2, 3, ..., K-1\,,
\end{aligned}
\tag{2.199}
$$

Recursion formula (2.199) can be used for generating polynomials $p_n(x)$ of degree up to $K-1$. Polynomials $p_n(x)$ of degrees greater or equal to K have roots at sampling points ξ^k [4]. Therefore, polynomial $p_n(x)$ of K^{th} degree

$$
p_K(x) = (x - \xi^1)(x - \xi^2)...(x - \xi^K) \tag{2.200}
$$

is determined by K discrete sampling points ξ^k as its roots.

Since polynomials $p_n(x)$ ($n \geq K$) have roots at sampling points ($p_n(\xi^k) = 0$ for all k) they satisfy the condition of orthogonality

$$
(\forall n \geq K) \quad \sum_{k=1}^{K} w^k h(\xi^k) \underbrace{p_n(\xi^k)}_{0} = 0\,, \tag{2.201}
$$

with respect to any function $h(x)$.

To apply developed formulas, it is convenient to introduce variables I_k^*, J_r^*, d_n^* and β_n already defined by (2.197) and (2.198). Therefore, by analogy to (2.58) the coefficients

$$
\begin{aligned}
b_n &= \frac{\langle x p_{n-1}, p_{n-1} \rangle}{\langle p_{n-1}, p_{n-1} \rangle} = \frac{1}{d_{n-1}^*} \sum_{r=0}^{n-1} \sum_{s=0}^{n-1} a_{n-1,r} a_{n-1,s} I_{r+s+1}^*\,, \\
c_{n-1} &= \frac{\langle p_{n-1}, p_{n-1} \rangle}{\langle p_{n-2}, p_{n-2} \rangle} = \frac{d_{n-1}^*}{d_{n-2}^*}\,,
\end{aligned}
\tag{2.202}
$$

can be calculated.

Complete procedure for calculating coefficients a_{nr} of orthogonal polynomials, coefficients β_n (2.198) and coefficients α_r (2.19) of resultant approximation polynomial $\tilde{f}(x, \alpha)$ (2.1) is given in Algorithm 2.7.

Algorithm 2.7. Coefficients α_r for the orthogonal polynomial approximation on a discrete domain – method 2

List of input variables: $N, K, \xi^k, w^k, f^k, \xi^k$

List of output variables: α_r

```
// Polynomial p_0(x) = 1                  // "//" denotes the beginning of a comment
    a_{0,0} = 1
    Calculate_and_store_sums I*_0, J*_0            // Equation (2.197)
    d*_0 = I*_0; β_0 = J*_0 / d*_0
// Polynomial p_1(x) = x - b_1
    Calculate_and_store_sums I*_1, I*_2, J*_1      // Equation (2.197)
    b_1 = I*_1 / d*_0
    a_{1,1} = 1; a_{1,0} = -b_1
    d*_1 = a_{1,0} I*_1 + I*_2; β_1 = (a_{1,0} J*_0 + J*_1) / d*_1     // Equation (2.198)
// Polynomials p_2(x), ..., p_{N-1}(x)
    for n = 2, ..., N-1
      Calculate_and_store_integrals I*_{2n-1}, I*_{2n}, J*_n   // Equation (2.197)
      b_n = Σ_{r=0}^{n-1} Σ_{s=0}^{n-1} a_{n-1,r} a_{n-1,s} I*_{r+s+1} / d*_{n-1}; c_{n-1} = d*_{n-1} / d*_{n-2}   // Eq. (2.198)
      // Coefficients a_{nr} of orthogonal polynomial p_n(x) (2.8)
        a_{n,0} = -b_n a_{n-1,0} - c_{n-1} a_{n-2,0}
        for r = 1, ..., n-2
          a_{nr} = a_{n-1,r-1} - b_n a_{n-1,r} - c_{n-1} a_{n-2,r}     // Equation (2.56)
        endfor
        a_{n,n-1} = a_{n,n-2} - b_n a_{n-1,n-1}; a_{nn} = a_{n-1,n-1}
      d*_n = Σ_{r=0}^{n} a_{nr} I*_{r+n}; β_n = Σ_{r=0}^{n} a_{nr} J*_r / d*_n   // Generalised Fourier coeff. (2.198)
    endfor
// Calculating coefficients α_r of approximation polynomial f~(x,α) (2.1)
    for r = 0, ..., N-1
      α_r = Σ_{n=r}^{N-1} β_n a_{nr}                       // Equation (2.19)
    endfor
end
```

2.5.3 Gram polynomials

Polynomials $P_n^K(x)$ ($n = 0, 1, ..., K-1$) that are orthogonal on the K sampling points

$$\xi^k = -1 + \frac{2(k-1)}{K-1}, \quad k = 1, 2, ..., K, \tag{2.203}$$

equally spaced on the interval $[-1,1]$ with respect to the unit weighting coefficients $w^k = 1$, are usually known as *Gram polynomials*[14] [12, 13].

The Gram polynomials can be expressed in the form

$$\begin{aligned} &P_n^K(x) = c_n^K \sum_{k=0}^{n} (-1)^k \frac{(n+k)^{(2k)}}{(k!)^2} \frac{s^{(k)}}{(K-1)^{(k)}}, \\ &s = \tfrac{1}{2}(x+1)(K-1). \end{aligned} \tag{2.204}$$

Herein upper index in the brackets denotes *factorial powers* $\alpha^{(k)}$ (B.1), as defined in the Appendix B.

Constants c_n^K can be chosen arbitrary to satisfy some criteria (e.g. to make polynomials orthonormal or to satisfy the condition $P_n^K(1) = 1$ $(n > K)$, etc.). The expanded form of expression (2.204) is

$$\begin{aligned} P_n^K(x) = c_n^K \Big(1 - \frac{(n+1)n}{(1!)^2} \frac{s}{K-1} + \frac{(n+2)(n+1)n(n-1)}{(2!)^2} \frac{s(s-1)}{(K-1)(K-2)} - \\ - \frac{(n+3)(n+2)(n+1)n(n-1)(n-2)}{(3!)^2} \frac{s(s-1)(s-2)}{(K-1)(K-2)(K-3)} + ... \Big). \end{aligned} \tag{2.205}$$

The recursion formula

$$P_n^K(x) = \frac{(2n-1)(K-1)}{n(K-n)} x P_{n-1}^K(x) - \frac{(n-1)(K+n-1)}{n(K-n)} P_{n-2}^K(x), \tag{2.206}$$

can be used for generating polynomials $P_n^K(x)$ of degree up to $K-1$. Polynomials $P_n^K(x)$ of degrees greater or equal to K have roots at sampling points ξ^k [4]. Therefore, polynomial $P_K^K(x)$ of K^{th} degree

$$P_K^K(x) = (x - \xi^1)(x - \xi^2)...(x - \xi^K) \tag{2.207}$$

is determined by K discrete sampling points ξ^k as its roots.

Example 2.11. First few Gram polynomials are

$$
\begin{aligned}
P_0^K &= 1, \\
P_1^K &= x, \\
P_2^K &= \frac{3(K-1)x^2-(K+1)}{2(K-2)}, \\
P_3^K &= \frac{15(K-1)^2x^3-[5(K^2-1)+4(K^2-4)]x}{6(K-3)(K-2)}.
\end{aligned}
\tag{2.208}
$$

Coefficients of Gram polynomials depend on the number of sampling points *K*. For five point approximation with Gram polynomials $K=5$. The relevant orthogonal polynomials of degrees zero through four can be obtained by adopting recursion formula (2.206):

$$P_n^5(x)=\frac{4(2n-1)}{n(5-n)}xP_{n-1}^5(x)-\frac{(n-1)(4+n)}{n(5-n)}P_{n-2}^5(x)\,. \tag{2.209}$$

Therefore, the first few Gram polynomials in five point approximation are

$$
\begin{aligned}
P_0^5 &= 1, \\
P_1^5 &= x, \\
P_2^5 &= 2x^2-1, \\
P_3^5 &= \tfrac{1}{3}(20x^3-17x), \\
P_4^5 &= \tfrac{1}{3}(140x^4-155x^2+18).
\end{aligned}
\tag{2.210}
$$

It may be seen that the *n*-th polynomial is an even function of *x* when *n* is even, and an odd function of *x* when *n* is odd. Also, each polynomial takes on the value *unity* when $x=1$ (i.e. $P_n^K(1)=1$).

Gram polynomials possess orthogonality property

$$\langle P_n^K, P_m^K\rangle=\sum_{k=1}^{K}P_n^K(\xi^k)P_m^K(\xi^k)\begin{cases}=0, & n\neq m,\\ \neq 0, & n<K.\end{cases} \tag{2.211}$$

If $n\geq K$, then $\langle P_n^K, P_n^K\rangle=0$.

When $n \ll K^{1/2}$, Gram polynomials are very similar to Legendre polynomials, but when $n \gg K^{1/2}$, they have very large oscillations between the sampling points. Related to this is the fact that when fitting the polynomial to *equidistant* data, degree *n* of applied polynomials should not be greater than about $K^{1/2}$ [12].

Further, if K is increased without limit then $P_n^K(x)$ tends to n^{th} degree Legendre polynomial $P_n(x)$:

$$\lim_{K\to\infty} P_n^K(x) = P_n(x)\,. \tag{2.212}$$

That can be easily verified by increasing K to infinity in recursion formula (2.206). The result is recursion formula (2.62) for Legendre polynomials.

2.5.4 Approximation with Gram polynomials

The $N-1^{\text{th}}$ degree least squares polynomial approximation of the function $f(x)$ over the K sampling points is given by

$$\tilde{f}(x,\beta) = \sum_{n=0}^{N-1} \beta_n P_n^K(x), \quad N < K, \tag{2.213}$$

where generalised Fourier coefficients are

$$\beta_n = \frac{\langle f, P_n^K \rangle}{\langle P_n^K, P_n^K \rangle} = \frac{\sum_{k=1}^{K} f(\xi^k) P_n^K(\xi^k)}{\sum_{k=1}^{K} [P_n^K(\xi^k)]^2}\,. \tag{2.214}$$

To apply developed formulas, it is convenient to introduce auxiliary variables

$$\begin{aligned} I_r^{\bullet} &= \sum_{k=1}^{K} (\xi^k)^r, \\ J_r^{\bullet} &= \sum_{k=1}^{K} f^k \cdot (\xi^k)^r. \end{aligned} \tag{2.215}$$

By analogy to equations (2.198) and (2.33) it can be obtained

$$\begin{aligned} d_n^{\bullet} &= \langle P_n^K, P_n^K \rangle = \langle P_n^K, x^n \rangle = \sum_{r=0}^{n} a_{nr} I_{r+n}^{\bullet}, \\ \beta_n &= \frac{\langle f, P_n^K \rangle}{\langle P_n^K, P_n^K \rangle} = \frac{1}{d_n^{\bullet}} \sum_{r=0}^{n} a_{nr} J_r^{\bullet}. \end{aligned} \tag{2.216}$$

Complete procedure for calculating coefficients a_{nr} (2.30) of Gram polynomials, coefficients β_n and coefficients α_r (2.19) of resultant approximation polynomial $\tilde{f}(x,\alpha)$ (2.1) is given in Algorithm 2.8.

Algorithm 2.8. Coefficients α_r in Gram polynomial approximation

List of input variables: N, K, f^k

List of output variables: α_r, β_n

// Equidistant sampling points ξ^k on the interval $[-1,1]$

for $k = 1, 2, ..., K$

$\xi^k = -1 + 2(k-1)/(K-1)$

endfor

$a_{0,0} = 1$ // Polynomial $P_0^K(x) = 1$

Calculate_and_store_sums $I_0^\bullet$, $J_0^\bullet$ // Equations (2.215)

$d_0^\bullet = I_0^\bullet$; $\beta_0 = J_0^\bullet / d_n^\bullet$ // Equations (2.216)

$a_{1,1} = 1$; $a_{1,0} = 0$ // Polynomial $P_1^K(x) = x$

Calculate_and_store_sums $I_1^\bullet$, $I_2^\bullet$, $J_1^\bullet$ // Equations (2.215)

$d_1^\bullet = I_2^\bullet$, $\beta_1 = J_1^\bullet / d_1^\bullet$ // Equations (2.216)

// Polynomials $P_2^K(x)$, …, $P_{N-1}^K(x)$

for $n = 2, ..., N-1$

Calculate_and_store_sums $I_{2n-1}^\bullet$, $I_{2n}^\bullet$, $J_n^\bullet$ // Equations (2.215)

// Calculate coefficients a_{nr} of $P_n^K(x)$ using recursion formula (2.206)

$a_{n,0} = -(n-1)(K+n-1)\, a_{n-2,0} / (n(K-n))$

for $r = 1, ..., n-2$

$$a_{nr} = \frac{(2n-1)(K-1)a_{n-1,r-1} - (n-1)(K+n-1)a_{n-2,r}}{n(K-n)}$$

endfor

$$a_{n,n-1} = \frac{(2n-1)(K-1)a_{n-1,n-2}}{n(K-n)}; \quad a_{nn} = \frac{(2n-1)(K-1)a_{n-1,n-1}}{n(K-n)}$$

$d_n^\bullet = \sum_{r=0}^{n} a_{nr} I_{r+n}^\bullet$; $\beta_n = \sum_{r=0}^{n} a_{nr} J_r^\bullet / d_n^\bullet$ // Equations (2.216)

endfor

// Calculate coefficients α_r of approximation polynomial $\tilde{f}(x,\alpha)$ (2.1)

for $r = 0, ..., N-1$

$\alpha_r = \sum_{n=r}^{N-1} \beta_n a_{nr}$ // Equation (2.19)

endfor

end

2.6 CONVERSION OF POWER SERIES

Exact integration in continuous approximation is usually avoided by using numeric integration or by using discrete approximation. Any type of integration can be completely avoided in continuous approximation method based on the conversion of power series. This method consists in

1. obtaining initial power series (e.g. by Maclaurin series expansion),
2. converting obtained power series into a series of orthogonal polynomials,
3. truncating polynomial series and in
4. converting truncated polynomials series back into a power series.

Obtained power series can be almost equal to those obtained in approximation with orthogonal polynomials on a continuous domain. The matching is better if a greater number of elements of initial power series is used.

Power series can be converted into a series of orthogonal polynomials by expansion of monomials x^m. Any monomial x^m of order m can be expanded with the first $m+1$ orthogonal polynomials $p_0(x), p_1(x), ..., p_m(x)$ by using equation

$$x^m = \sum_{n=0}^{m} c_{mn} p_n(x)\,. \tag{2.217}$$

By substituting polynomial $p_n(x)$ (2.8) it follows

$$x^m = \sum_{n=0}^{m}\left(c_{mn} \sum_{r=0}^{n} a_{nr} x^r \right). \tag{2.218}$$

By rearranging that expression it can be obtained

$$\sum_{r=0}^{m}\left(\sum_{n=r}^{m} c_{mn} a_{nr} - \delta_{mn} \right) x^r = 0\,. \tag{2.219}$$

That equation is satisfied if and only if

$$(\forall r = 0, 1, ..., m)\ \sum_{n=r}^{m} c_{mn} a_{nr} = \delta_{rm}\,, \tag{2.220}$$

or

$$\begin{vmatrix} a_{0,0} & a_{1,0} & a_{2,0} & \dots & a_{m,0} \\ 0 & a_{1,1} & a_{2,1} & \dots & a_{m,1} \\ 0 & 0 & a_{2,2} & \dots & a_{m,2} \\ \dots & \dots & \dots & & \dots \\ 0 & 0 & 0 & \dots & a_{mm} \end{vmatrix} \begin{Bmatrix} c_{m,0} \\ c_{m,1} \\ \dots \\ c_{m,m-1} \\ c_{mm} \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ \dots \\ 0 \\ 1 \end{Bmatrix}. \tag{2.221}$$

Therefore, coefficients c_{mn} of expansion (2.117) can be easily calculated by recursion

$$
\begin{aligned}
&c_{mm} = 1/a_{mm}, \\
&(\forall r = m-1, m-2, ..., 0)\;\; c_{mr} = \frac{-1}{a_{rr}} \sum_{n=r+1}^{m} c_{mn} a_{nr}.
\end{aligned}
\tag{2.222}
$$

It should be noted that recursion is carried out in reverse order, from $r = m-1$ to $r = 0$.

If orthogonal polynomials $p_n(x)$ are standardised so that $p_n(x) = x^n + ...$ (i.e., the leading coefficients a_{nn} have value 1), the diagonal elements of matrix in equation (2.221) take unit values, so that

$$
\begin{vmatrix}
1 & a_{1,0} & a_{2,0} & ... & a_{m,0} \\
0 & 1 & a_{2,1} & ... & a_{m,1} \\
0 & 0 & 1 & ... & a_{m,2} \\
... & ... & ... & & ... \\
0 & 0 & 0 & ... & 1
\end{vmatrix}
\begin{Bmatrix} c_{m,0} \\ c_{m,1} \\ ... \\ c_{m,m-1} \\ c_{mm} \end{Bmatrix}
=
\begin{Bmatrix} 0 \\ 0 \\ ... \\ 0 \\ 1 \end{Bmatrix},
\tag{2.223}
$$

while the recursion (2.222) simplifies to

$$
\begin{aligned}
&c_{mm} = 1, \\
&(\forall r = m-1, m-2, ..., 0)\;\; c_{mr} = -\sum_{n=r+1}^{m} c_{mn} a_{nr}.
\end{aligned}
\tag{2.224}
$$

If the initial power series is infinite, it has a form

$$
f(x,a) = \sum_{m=0}^{\infty} a_m x^m \, , \tag{2.225}
$$

which is equal to

$$
\begin{aligned}
&\sum_{m=0}^{\infty} a_m \sum_{n=0}^{m} c_{mn} p_n(x) = \\
&= \left(\sum_{m=0}^{\infty} a_m c_{m,0} \right) p_0(x) + \left(\sum_{m=1}^{\infty} a_m c_{m,1} \right) p_1(x) + \left(\sum_{m=2}^{\infty} a_m c_{m,2} \right) p_2(x) + ... \qquad (2.226) \\
&= \sum_{n=0}^{\infty} \left(\sum_{m=n}^{\infty} a_m c_{mn} \right) p_n(x),
\end{aligned}
$$

then the coefficients of resulting series $f(x,\beta)$ (2.7):

$$\beta_n = \sum_{m=n}^{\infty} a_m c_{mn} \tag{2.227}$$

are equal to the generalised Fourier coefficients β_n (2.10), or to those that can be obtained by the polynomial least-squares approximation applied to the $f(x)$.

In other words, if the initial power series is infinite and obtained by Maclaurin series expansion of function $f(x)$, the resultant series of orthogonal polynomials is the same as those obtained by applying orthogonal polynomials or polynomial least--squares method directly to the function $f(x)$.

The problem arises from the fact that coefficients β_n in (2.227) are defined as infinite sum. In practice, only the first *M* elements of initial power series $f(x,a)$ (2.225) are taken into account, so the calculation of coefficients β_n becomes finite. Therefore, in the resulting series

$$\tilde{f}(x,\tilde{\beta}) = \sum_{n=0}^{N-1} \tilde{\beta}_n p_n(x), \quad N \le M \ , \tag{2.228}$$

the generalised Fourier coefficients β_n (2.227) are approximated with

$$\tilde{\beta}_n = \sum_{m=n}^{M-1} a_m c_{mn} \ , \quad n = 0, 1, 2, ..., N-1 \ . \tag{2.229}$$

Finally, the coefficients α_r of polynomial $\tilde{f}(x,\alpha)$ (2.1) that is equivalent to approximation $\tilde{f}(x,\tilde{\beta})$ (2.228) can be calculated by using the formula (2.19) or, more precisely, by using the formula

$$\alpha_r = \sum_{n=r}^{N-1} \tilde{\beta}_n a_{nr} \ . \tag{2.230}$$

Procedure for calculating generalised Fourier coefficients $\tilde{\beta}_n$ and coefficients α_r of converted power series is presented in Algorithm 2.9.

The described procedure is frequently used in conversion of initial polynomial that approximates function $f(x)$ (usually contains the first *M* elements of Maclaurin series expansion) into series of *Chebyshev polynomials* (Chapter 4.). The obtained series is truncated and after that converted back into power series.

Although the resulting polynomial has lower degree than the initial one, the degradation of accuracy is usually minimal. Since the number of numerical operations required for calculating the values of approximated function for certain argument is reduced, the described conversion of polynomials is called *Chebyshev economisation* and it is described in Chapter 4.7.

Algorithm 2.9. Conversion of power series

List of input variables: M, N, a_m, a_{nr}
// M Number of summation elements of initial power series
// N Number of summation elements of converted power series ($N \le M$)
// a_m Coefficients of initial power series (or initial approximation)
// a_{nr} Coefficients of orthogonal polynomials $p_n(x)$

List of output variables: α_r , $\tilde{\beta}_n$ // "//" denotes the beginning of the comment

// Calculate coefficients c_{mr} (expansion of monomials x^m)
for $m = 0, 1, ..., M-1$
$c_{mm} = 1/a_{mm}$
for $r = \min(m-1, N-1), ..., 0$
$$c_{mr} = \frac{-1}{a_{rr}} \sum_{n=r+1}^{m} c_{mn} a_{nr}$$ // Equation (2.222)
endfor
endfor

// Calculate generalised Fourier coefficients
for $n = 0, 1, ..., N-1$
$$\tilde{\beta}_n = \sum_{m=n}^{M-1} a_m c_{mn}$$ // Equation (2.229)
endfor

// Calculate coefficients α_r of converted power series $\tilde{f}(x, \alpha)$ (2.1)
for $r = 0, ..., N-1$
$$\alpha_r = \sum_{n=r}^{N-1} \tilde{\beta}_n a_{nr}$$ // Equation (2.230)
endfor
end